



# Microscopie de force dynamique: éléments (Deuxième partie)

Laurent Nony

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# Microscopie à Force Atomique (AFM) en mode dynamique: éléments Deuxième partie

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*Séminaire interne, Juin 2006*

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UMR 6242 CNRS, Universités Paul Cézanne, Provence et Sud Toulon-Var



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SCIENTIFIQUE



# Introduction au non-contact AFM (ou FM-AFM)

Non-contact

Tapping

Modélisation

Introduction

nc-AFM vs. “Tapping” ou modulation de fréquence vs. modulation d’amplitude

Réelle méthode de non-contact

Sensibilité verticale très supérieure au “Tapping”

Méthode de découplage efficace des forces conservatives et dissipatives (pourvu que la phase soit bien maintenue)

Affranchissement de la constante de temps liée au facteur de qualité

Technique essentiellement UHV (requiert  $Q$  élevé)

**Contribution potentielle de l’électronique aux signaux de mesure !**

# Le non-contact AFM

Non-contact

Tapping

Modélisation

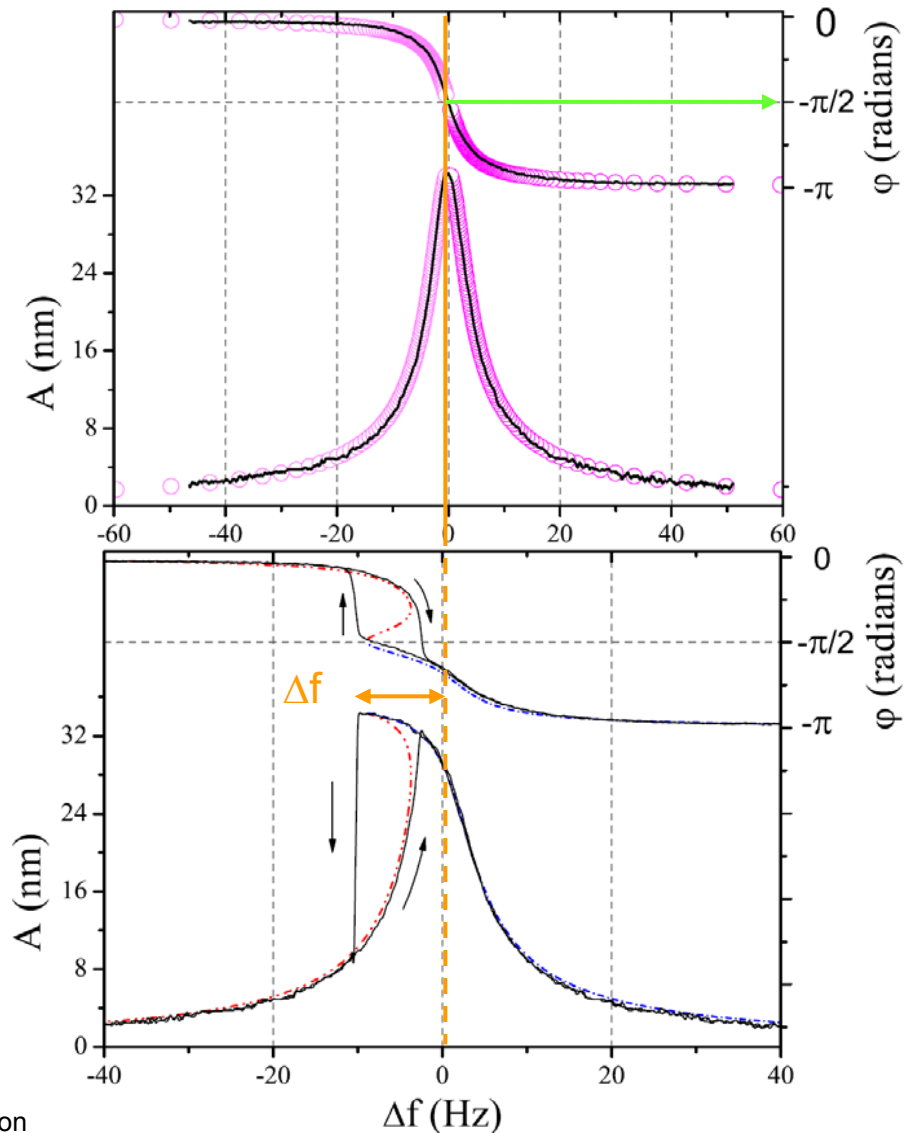
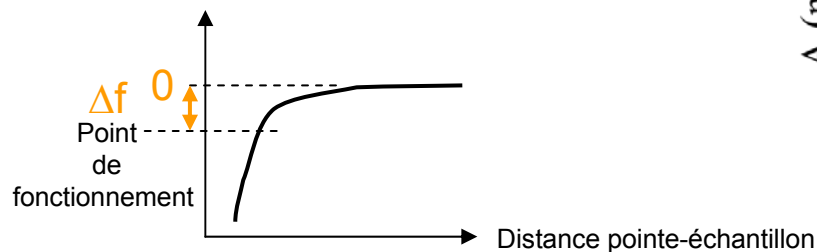
Introduction

Phase fixée ( $= -90^\circ$ ) et  
amplitude d'oscillation fixée  
(modulation de fréquence)



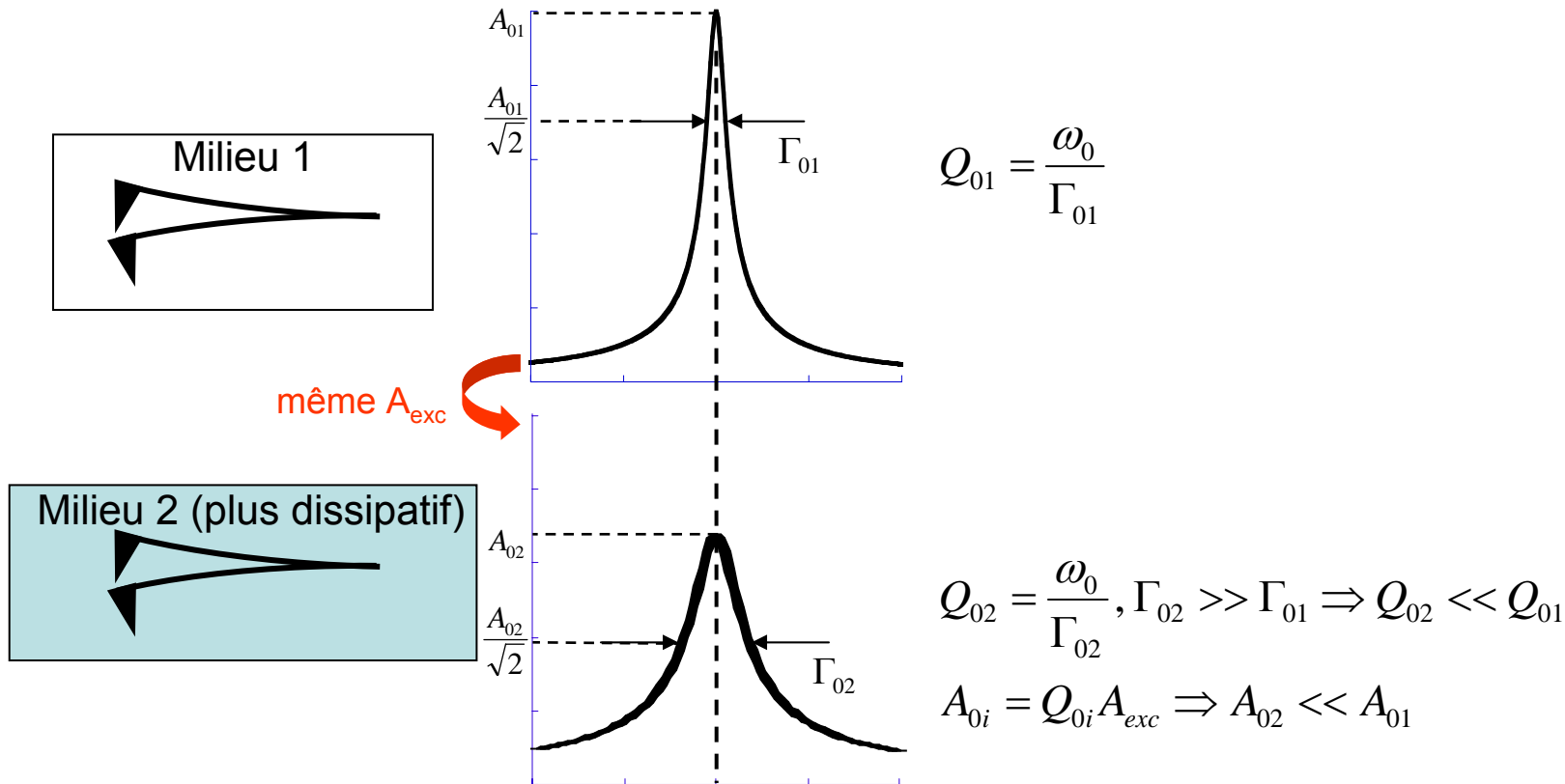
Mesures : décalage de la fréquence  
de résonance et amplitude  
d'excitation requise pour conserver  
l'amplitude d'oscillation constante  
en fonction de la distance pointe-  
surface

Asservissement : décalage donné de la  
fréquence de résonance



# Mesure d'effets dissipatifs en nc-AFM

- Energie dissipée par un oscillateur harmonique



$$Q = 2\pi \frac{\langle E_{stored} \rangle_T}{\langle E_{diss} \rangle_T} \Leftrightarrow \langle E_{diss} \rangle_T = 2\pi \frac{\langle E_{stored} \rangle_T}{Q} \Rightarrow \langle E_{diss} \rangle_T = \pi \frac{kA_0^2}{Q} = \pi k A_0 A_{exc} = \pi \frac{kA_0^2 \Gamma_0}{\omega_0}$$

$$A_{exc} \propto \langle E_{diss} \rangle_T \propto \Gamma_0$$

# Mesure d'effets dissipatifs en nc-AFM

- Le cas du nc-AFM :

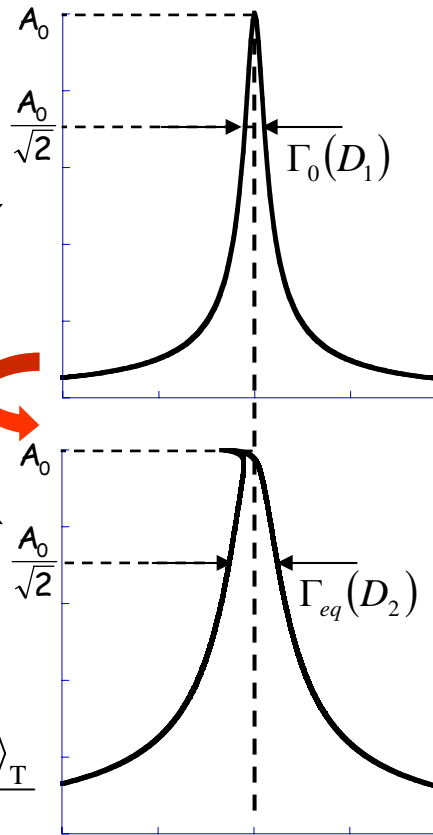
Vertical distance

$D_1$

$D_2$



$A_{exc}$  variée



$$Q_0(D_1) = \frac{\omega_0}{\Gamma_0(D_1)}$$

$$Q_{eq}(D_2) = \frac{\omega_0^{nl}}{\Gamma_{eq}(D_2)} \approx \frac{\omega_0}{\Gamma_0 + \Gamma_{int}},$$

avec  $\Gamma_{eq} > \Gamma_0$ , donc  $Q_{eq} < Q_0$

$$Q_{eq} = 2\pi \frac{\langle E_{stored} \rangle_T}{\langle E_{diss} \rangle_T}$$

En nc-AFM,  $A_0$  étant constante  $\rightarrow$  mesure de la dissipation en non-contact

$$\langle E_{diss} \rangle_T = \pi k A_0 A_{exc} = \pi \Gamma_{eq}(D) \frac{k_0 A_0^2}{\omega_0} \Rightarrow$$

Les variations de  $A_{exc}$  pour conserver  $A_0$  constante forment une image de "dissipation (ou damping)"

Ordres de grandeur (@RT) :

$$\begin{aligned} k &= 30 \text{ N/m} \\ A_0 &= 10 \text{ nm} \\ A_{exc} &= A_0/Q = 10/30000 \sim 0.3 \text{ pm} \end{aligned} \quad \langle E_{diss} \rangle_T = 2 \text{ eV/cycle}$$

# Illustrations expérimentales

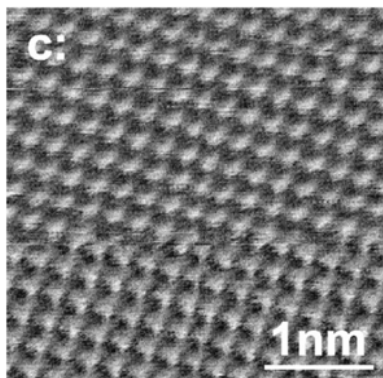
Non-contact

Tapping

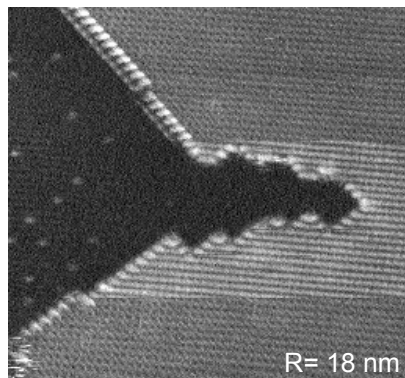
Modélisation

Introduction

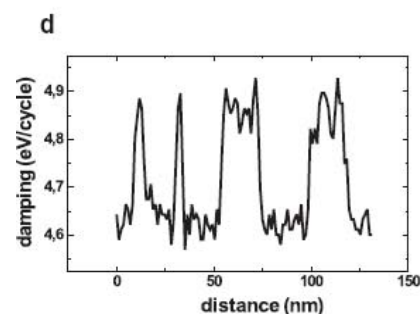
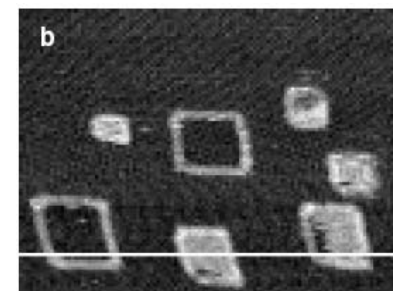
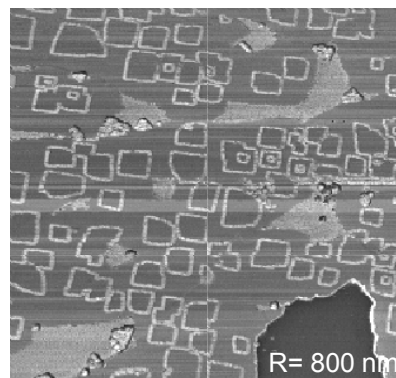
- Signal de dissipation (contrôle sur le  $\Delta f$ ) :



Cu(100)

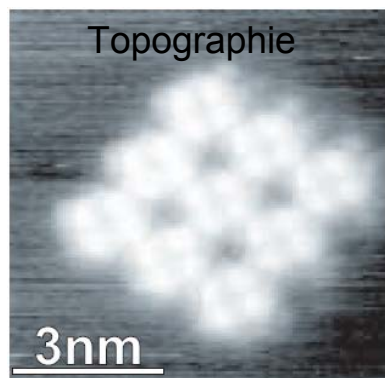


NaCl / Cu(111)

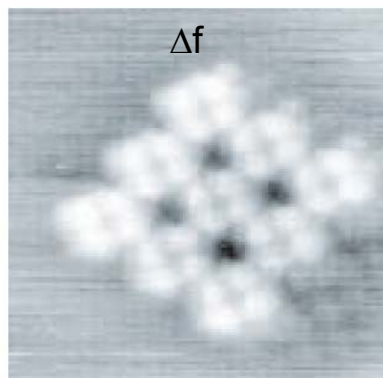


KBr+e-+PTCDA

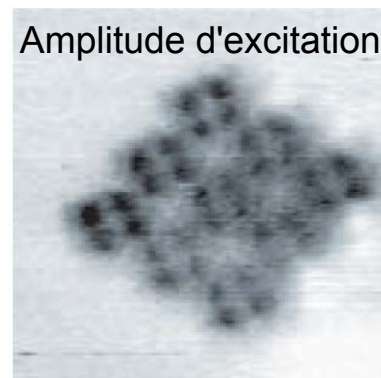
- Contrôle sur courant tunnel :



Topographie



$\Delta f$



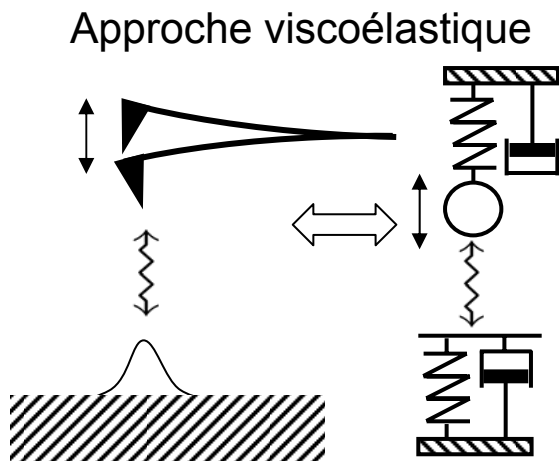
Amplitude d'excitation

Porphyrines sur Cu(100)



# Problématique actuelle en nc-AFM

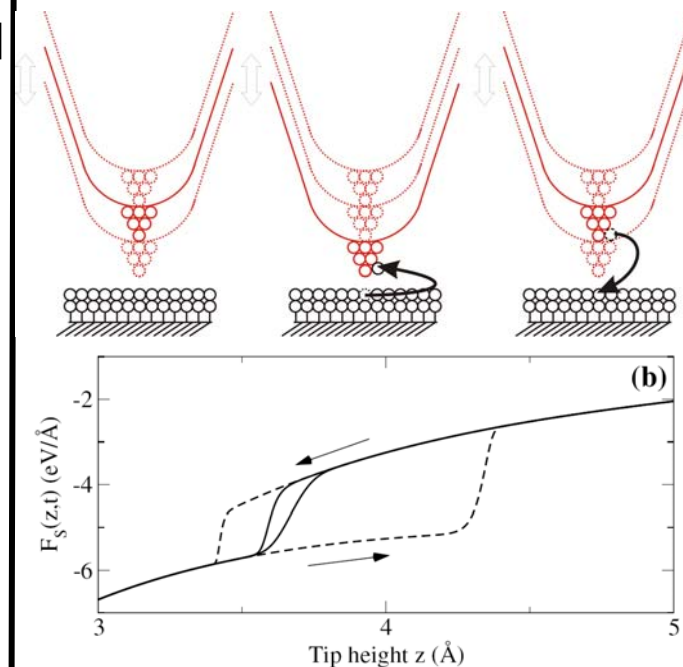
- Dissipation à l'échelle atomique : **canaux de dissipation** ?



Terme de couplage :  
force d'interaction

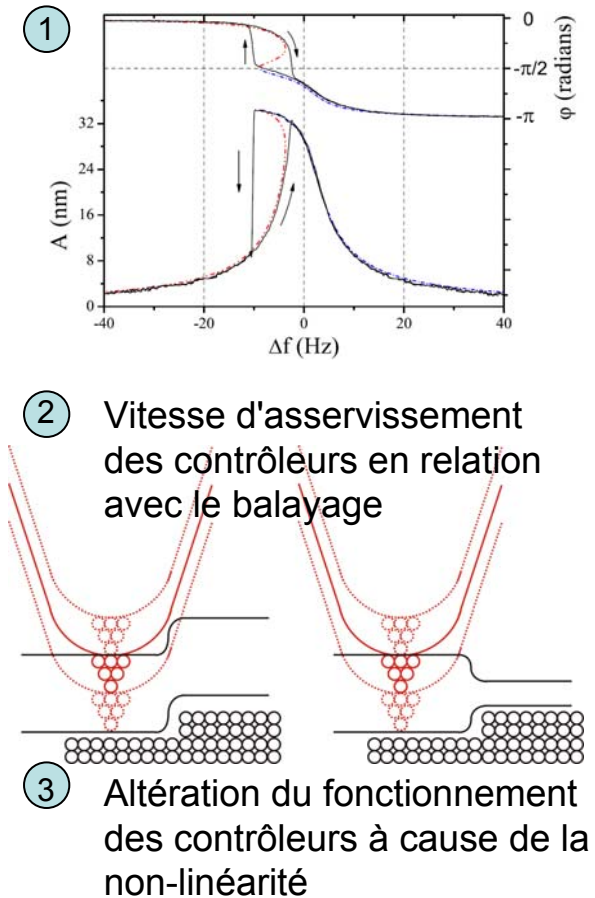
Approche continue : OK sur  
des polymères (300 kHz), mais  
à l'échelle atomique?

Instabilités atomiques  
(hystérésis d'adhésion)



Ordres de grandeurs compatibles avec  
les résultats expérimentaux.  
Mais s'il n'existe pas de "mode mou"  
en surface (défaut, marche)?

Rôle de l'instrumentation  
**Dissipation apparente**



**Dans tous les cas : dissipation induite par le régime attractif**



# Problématique actuelle en nc-AFM

PRL 97, 016103 (2006)

PHYSICAL REVIEW LETTERS

week ending  
7 JULY 2006

## Identification of Nanoscale Dissipation Processes by Dynamic Atomic Force Microscopy

R. Garcia,<sup>1,\*</sup> C. J. Gómez,<sup>1</sup> N. F. Martinez,<sup>1</sup> S. Patil,<sup>1</sup> C. Dietz,<sup>2</sup> and R. Magerle<sup>2</sup>

<sup>1</sup>*Instituto de Microelectrónica de Madrid, CSIC, Isaac Newton 8, 28760 Tres Cantos, Madrid, Spain*

<sup>2</sup>*Chemische Physik, Technische Universität Chemnitz, D-09107 Chemnitz, Germany*

(Received 11 April 2006; published 7 July 2006)

Identification of energy-dissipation processes at the nanoscale is demonstrated by using amplitude-modulation atomic force microscopy. The variation of the energy dissipated on a surface by a vibrating tip as a function of its oscillation amplitude has a shape that singles out the dissipative process occurring at the surface. The method is illustrated by calculating the energy-dissipation curves for surface energy hysteresis, long-range interfacial interactions and viscoelasticity. The method remains valid with independency of the amount of dissipated energy per cycle, from 0.1 to 50 eV. The agreement obtained between theory and experiments performed on silicon and polystyrene validates the method.

# A nc-AFM simulator with PLL-controlled frequency detection and excitation : addressing the problem of apparent dissipation

L. Nony, A. Baratoff, D. Schär, A. Wetzel, O. Pfeiffer,  
R. Bennewitz\* and E. Meyer

June 2004

*NCCR on Nanoscale Science,  
Institute of Physics, Basel, Switzerland*

*\* Mc Gill University, Montreal, Canada*

# Motivations

Why a virtual machine?

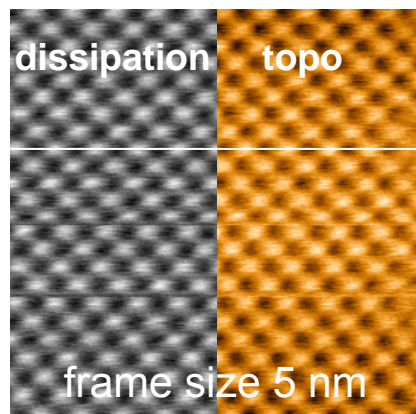
- Assessing the contribution of the instrumentation to the measurements
  - **apparent dissipation**
  - what component, how...
  - time constants of the system, establishing a hierarchy

Results

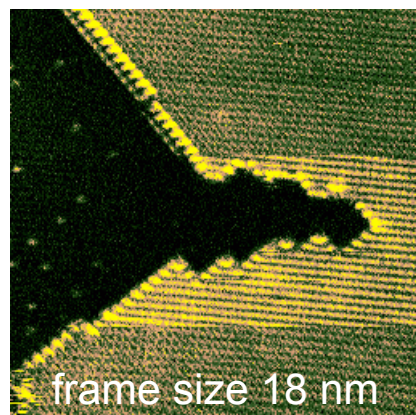
Description

Introduction

# Dissipation vs. apparent dissipation



topography and dissipation are neither correlated nor anti-correlated



Enhanced dissipation at steps  
(100 meV/cycle)

VOLUME 89, NUMBER 14

PHYSICAL REVIEW LETTERS

30 SEPTEMBER 2002

## Interplay between Nonlinearity, Scan Speed, Damping, and Electronics in Frequency Modulation Atomic-Force Microscopy

Michel Gauthier,<sup>1</sup> Ruben Pérez,<sup>2</sup> Toyoko Arai,<sup>3</sup> Masahiko Tomitori,<sup>3</sup> and Masaru Tsukada<sup>1</sup>

<sup>1</sup>Department of Physics, Graduate School of Science, University of Tokyo, Hongo 7-3-1, Bunkyo-ku, Tokyo 113-0033, Japan

<sup>2</sup>Departamento de Física Teórica de la Materia Condensada, Universidad Autónoma de Madrid, E-28049 Madrid, Spain

<sup>3</sup>School of Materials Science, Japan Advanced Institute of Science and Technology,

1-1 Asahidai, Tatsunokuchi, Nomi-gun, Ishikawa 923-1292, Japan

(Received 23 March 2002; published 16 September 2002)

Numerical simulations of the frequency modulation atomic force microscope, including the whole dynamical regulation by the electronics, show that the cantilever dynamics is conditionally stable and that there is a direct link between the frequency shift and the conservative tip-sample interaction. However, a soft coupling between the electronics and the nonlinearity of the interaction may significantly affect the damping. A resonance between the scan speed and the response time of the system can provide a simple explanation for the spatial shift and contrast inversion between topographical and damping images, and for the extreme sensitivity of the damping to a tip change.

REVIEW OF SCIENTIFIC INSTRUMENTS

VOLUME 74, NUMBER 5

MAY 2003

## Noncontact atomic force microscopy: Stability criterion and dynamical responses of the shift of frequency and damping signal

G. Couturier,<sup>a)</sup> R. Boisgard, L. Nony,<sup>b)</sup> and J. P. Aimé

Centre de Physique Moléculaire Optique et Hertzienne, Université Bordeaux I, UMR5798 CNRS, 351 Cours de la Libération, 33405 Talence Cedex, France

(Received 23 July 2002; accepted 13 January 2003)

# Motivations

Why a virtual machine?

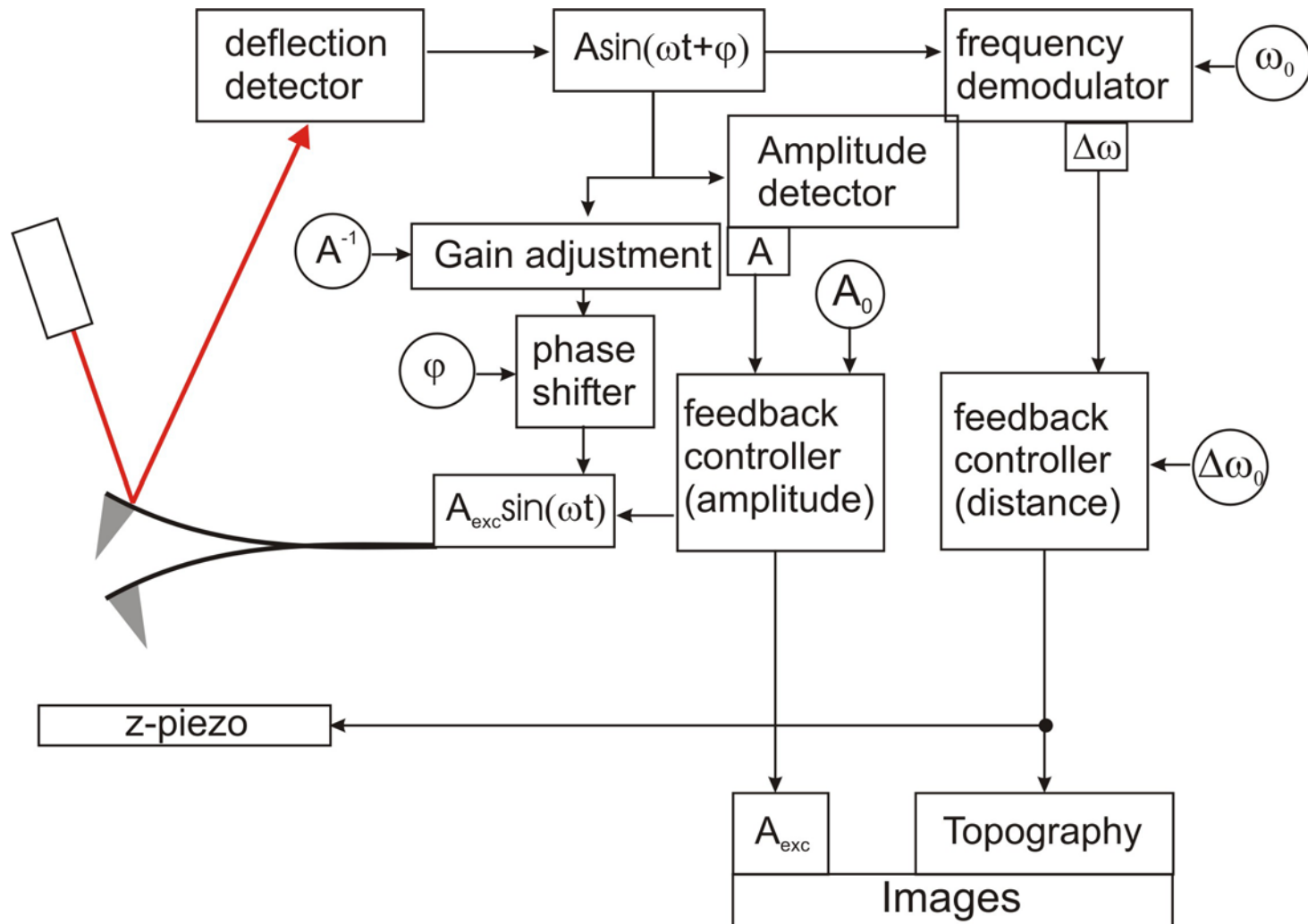
- Assessing the contribution of the instrumentation to the measurements
  - **apparent dissipation**
  - what component, how...
  - time constants of the system, establishing a hierarchy
- Doing physics
  - tip/surface interaction
  - dissipative processes
  - images calculation

Results

Description

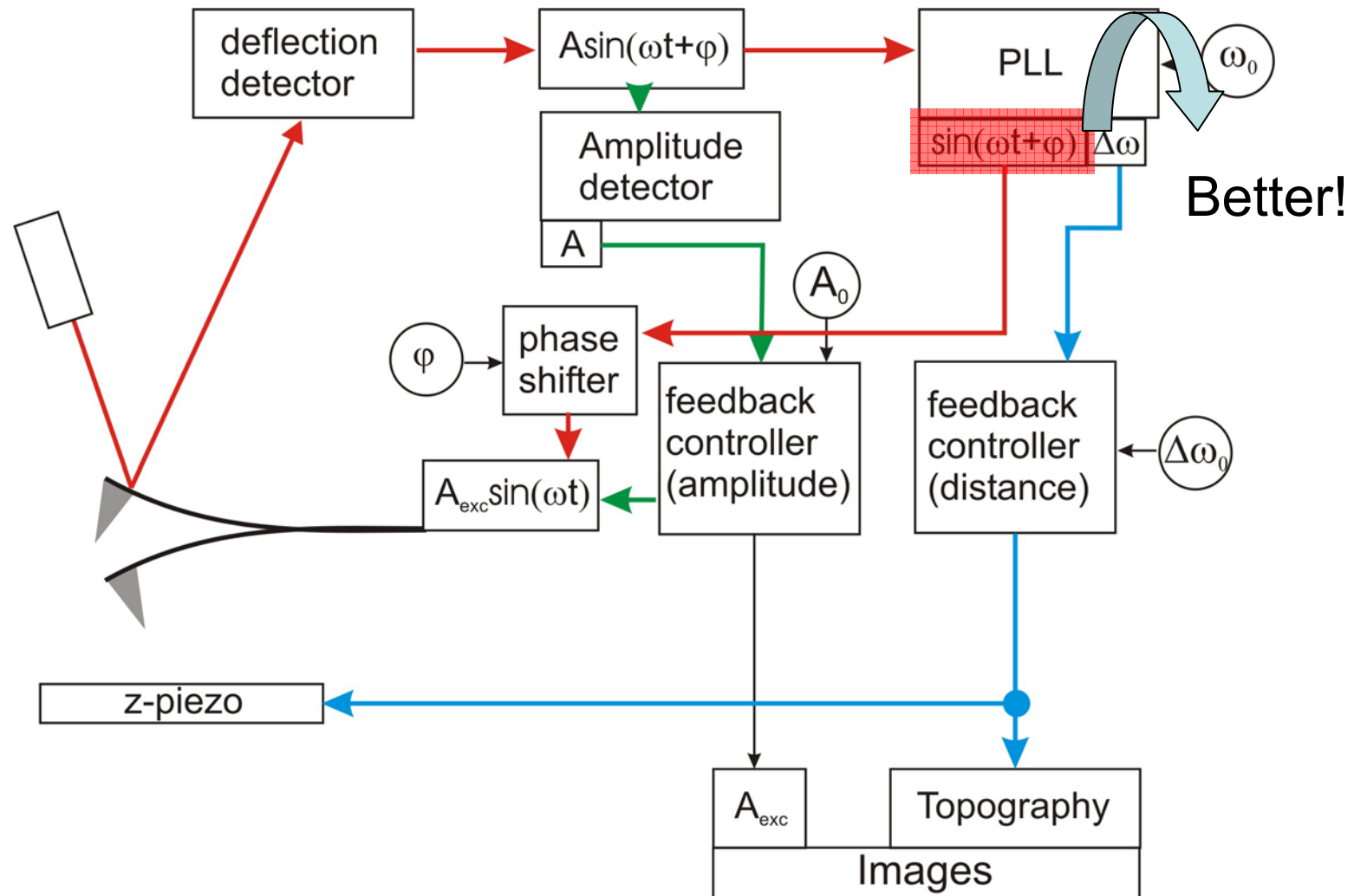
Introduction

# nc-AFM electronics : self-excitation scheme

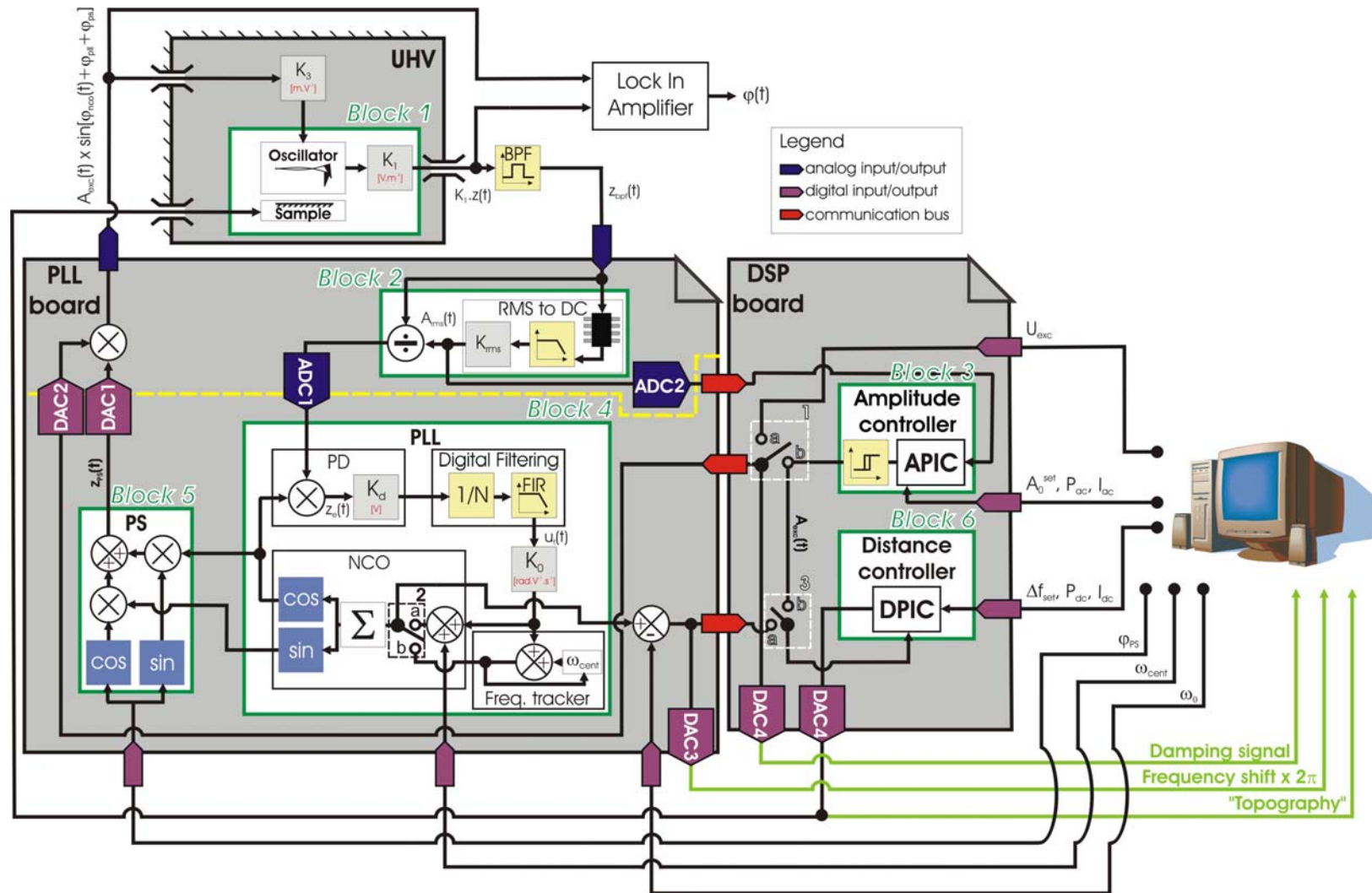




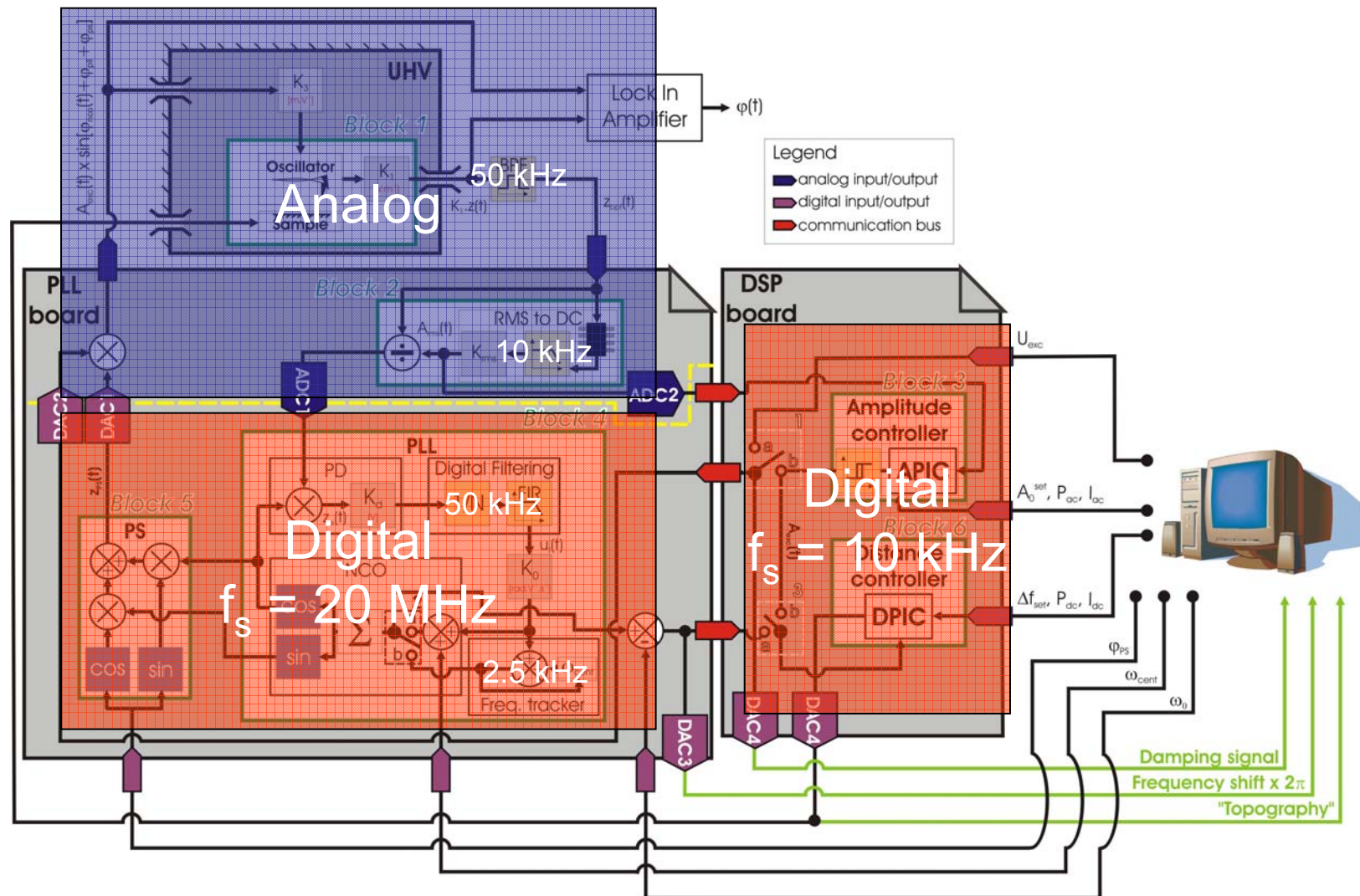
# nc-AFM electronics : self-excitation scheme



# Block diagram of the electronics



# Block diagram of the electronics



# Features

- Description of the real setup (mix of analog/digital devices)
- LabView™ implementation (now C version available)
- GUI with tunable parameters at run time
- The Phase-Locked Loop (PLL) detects the frequency shift and provides the excitation signal to the cantilever

Results

Description

Introduction

# Implementation

## ➤ Difficulties :

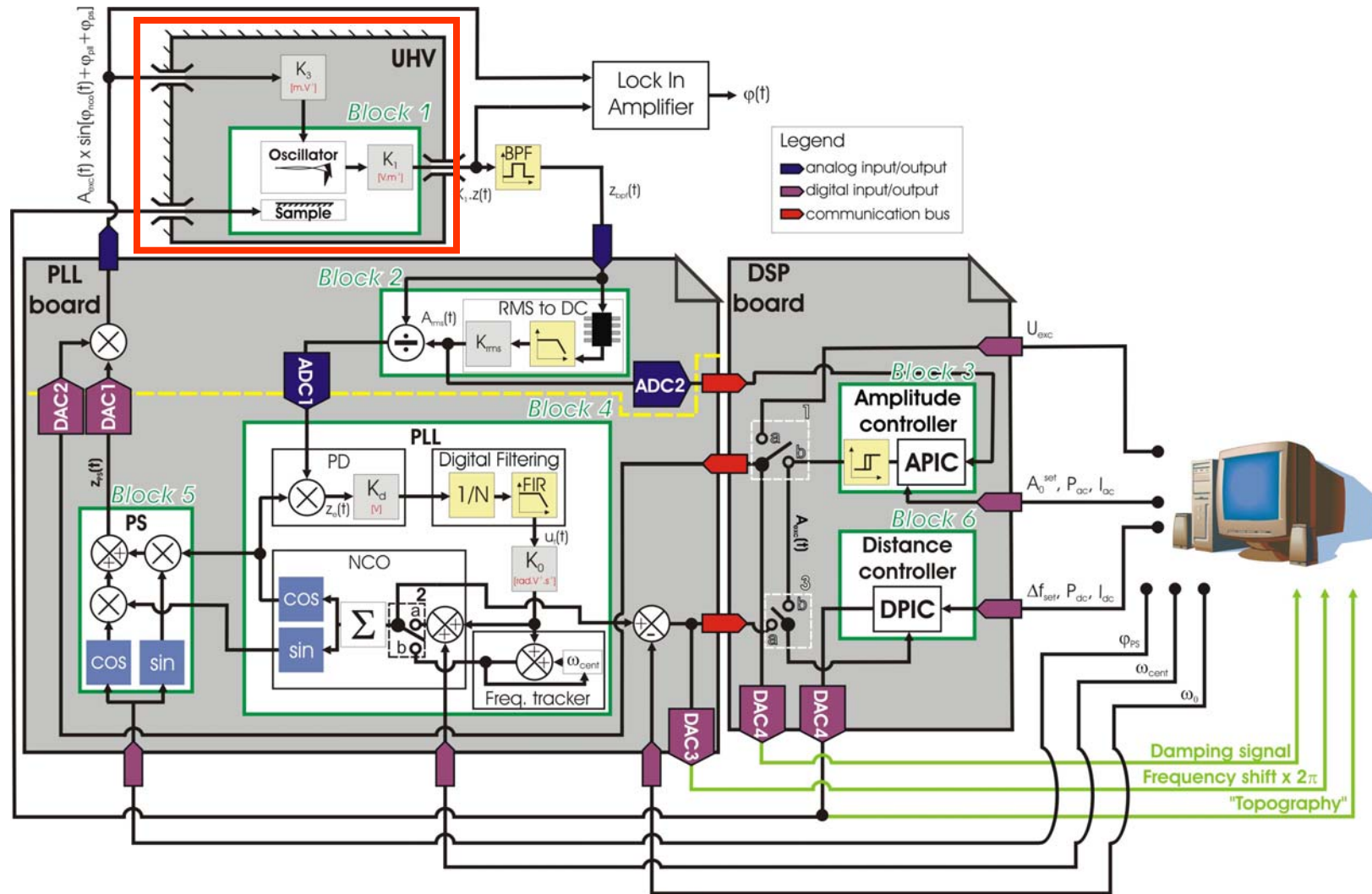
- Three (four) feedback loops: PLL, APIC, DPIC
- Various operating frequencies (many time constants)
- 3 controllers : 6 gains
- Non-linear problem with coupled components

## ➤ Assumptions :

- Analog components are solved with a modified Verlet's algorithm ( $f_s = 400$  MHz)
- DACs and ADCs are “ideal” components
- PSD and preamp. not described
- No noise
- Any physical channel of dissipation is considered

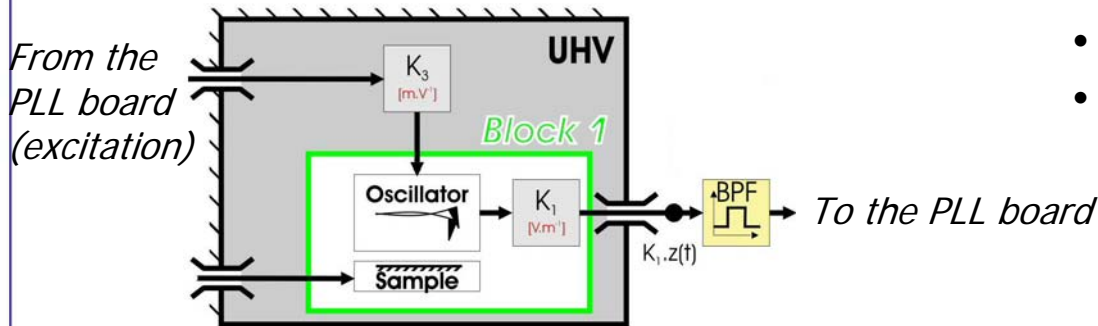


# Block diagram of the electronics





# Block 1, the oscillator



- Analog device
- $f_s = f_{s_0} = 200 \text{ MHz}$

Implementation :

$$\ddot{z}(t) + \frac{\omega_0}{Q}\dot{z}(t) + \omega_0^2 z(t) = \omega_0^2 \underline{A_{\text{exc}}(t)} + \frac{\omega_0^2 \underline{F_{\text{int}}(t)}}{k_c}$$

$$\underline{A_{\text{exc}}(t_i) = K_3 \times \underline{D_{\text{amp}}(t_i)} \times \underline{z_{\text{ps}}(t_i)}}$$

10 kHz
20 MHz

$$\underline{F_{\text{int}}(t) = -\partial_{r(t)} V_{\text{int}}(r(t))}$$

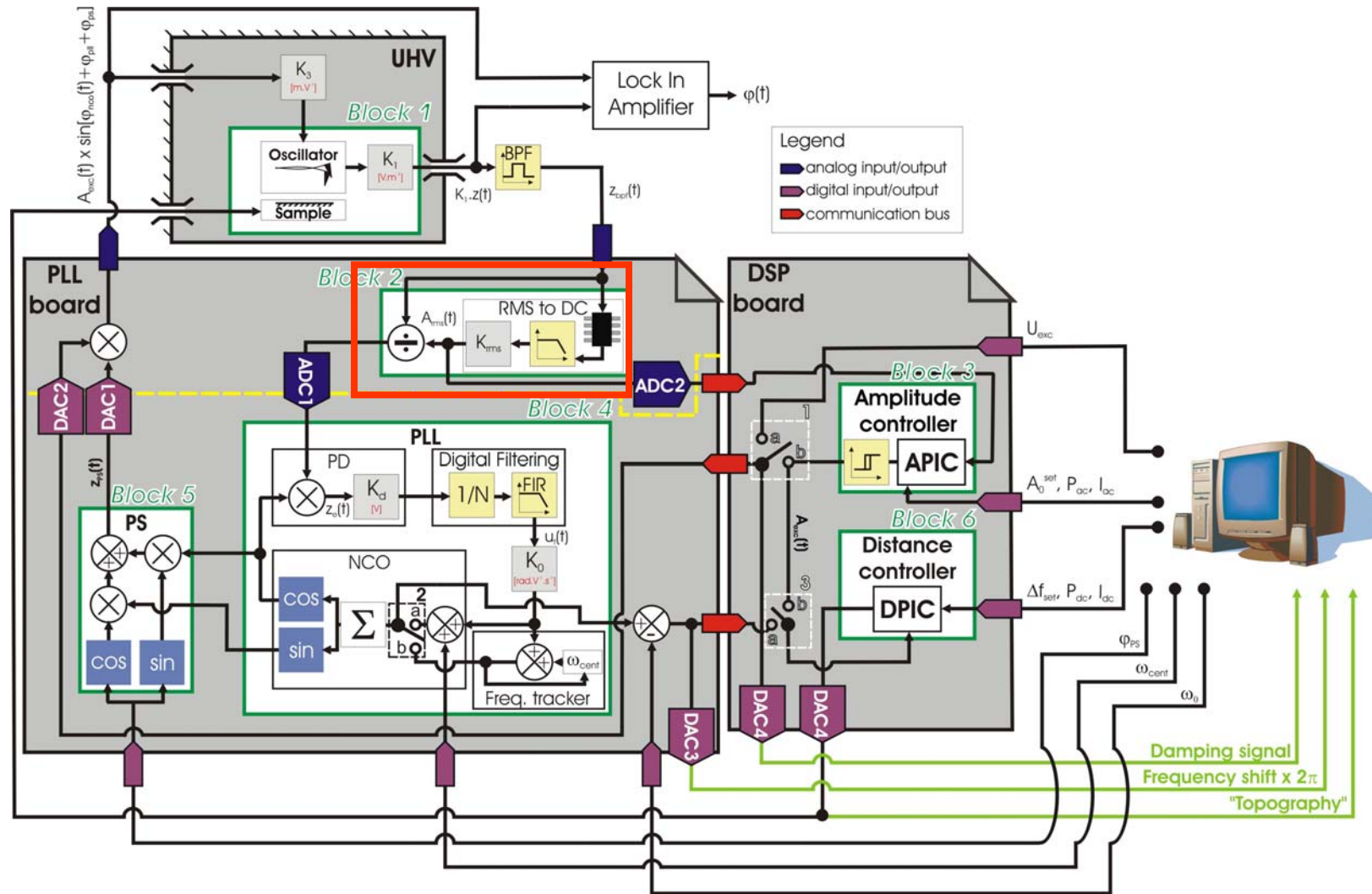
$$\begin{cases} V_{\text{int}}(r) = -\frac{HR}{6r} - U_0 \left[ 2e^{-\frac{r-r_c}{\lambda}} - e^{-\frac{2(r-r_c)}{\lambda}} \right] \\ r(t_i) = D(t_i) - z(t_i) \end{cases}$$

BPF output :

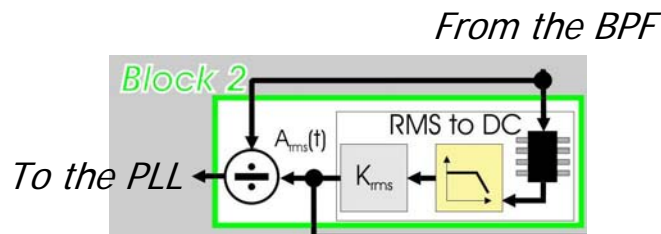
$$\ddot{z}_{\text{bpf}}(t) + 2\pi B_W \dot{z}_{\text{bpf}}(t) + \omega_c^2 z_{\text{bpf}}(t) = 2\pi B_W \times K_1 \times \dot{z}(t)$$

↪ 50 kHz

# Block diagram of the electronics



# Block 2, the RMS-to-DC converter



- Analog device (PLL board)
- $f_s = f_{s_0} = 200$  MHz

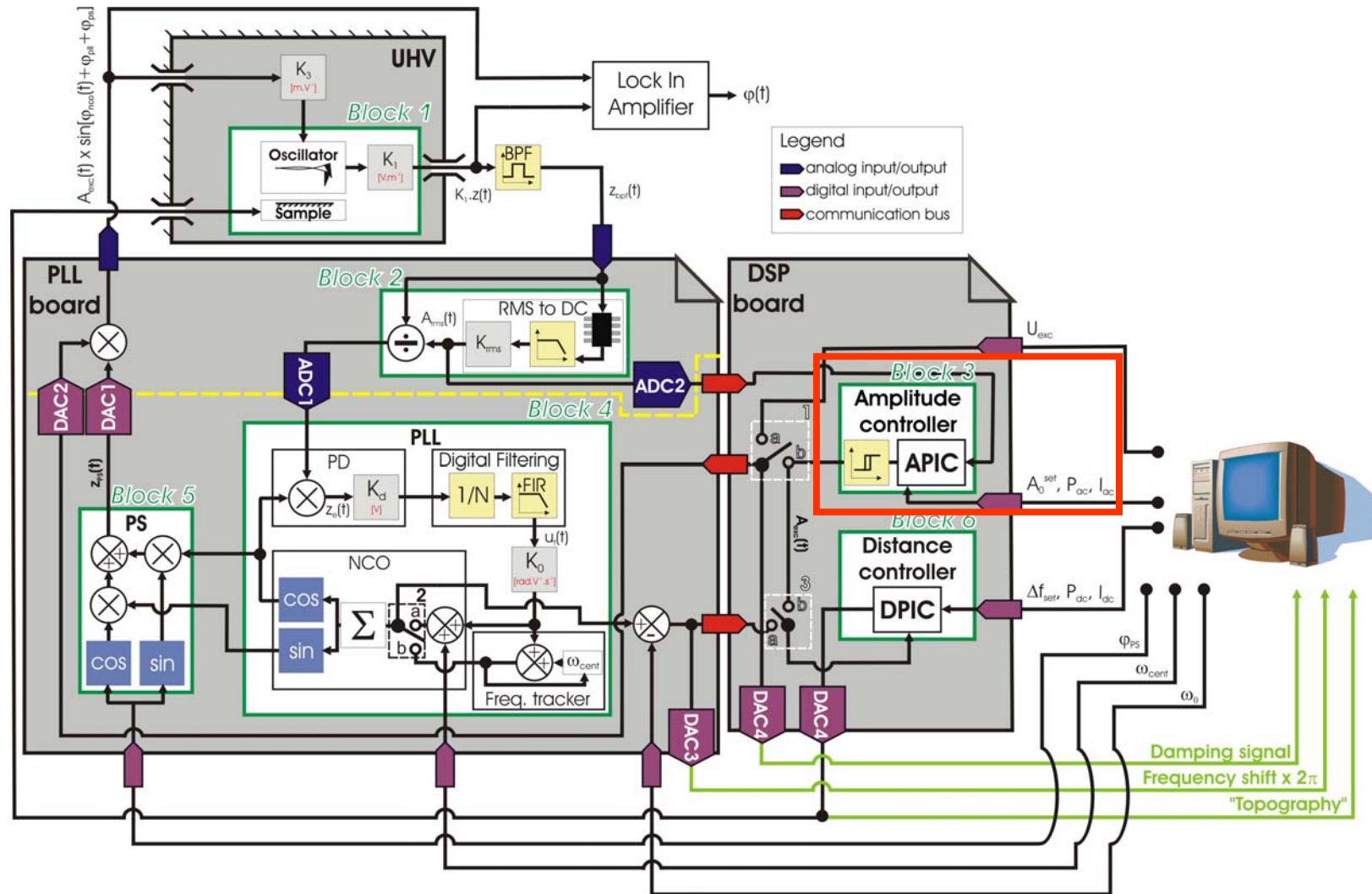
Implementation :

$$\begin{cases} A_{\text{rms}}(t_i) = K_{\text{rms}} \times \sqrt{V_s(t_i)} \\ \tau_{\text{rms}} \dot{V}_s(t) + V_s(t) = V_e(t) \Rightarrow \tau_{\text{rms}} = 15.9 \mu\text{s} (f_{\text{co}}^{\text{lp}} = 10 \text{ kHz}) \\ V_e(t_i) = z_{\text{bpf}}^2(t_i) \end{cases}$$

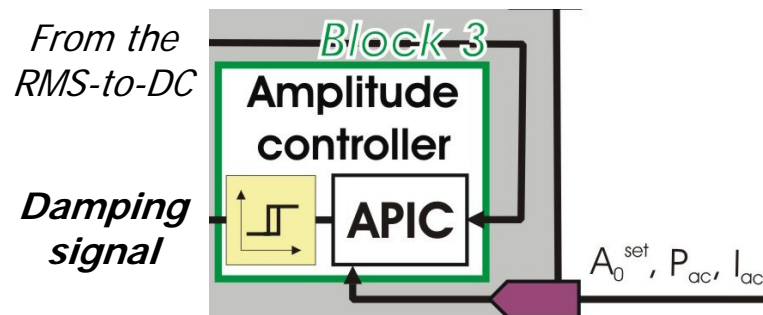
The PLL receives :

$$\frac{z_{\text{bpf}}(t_i)}{A_{\text{rms}}(t_i)}$$

# Block diagram of the electronics



# Block 3, the amplitude controller (APIC)



- Digital device (DSP board)
- Provides the output signal @  $f_s = 10$  kHz

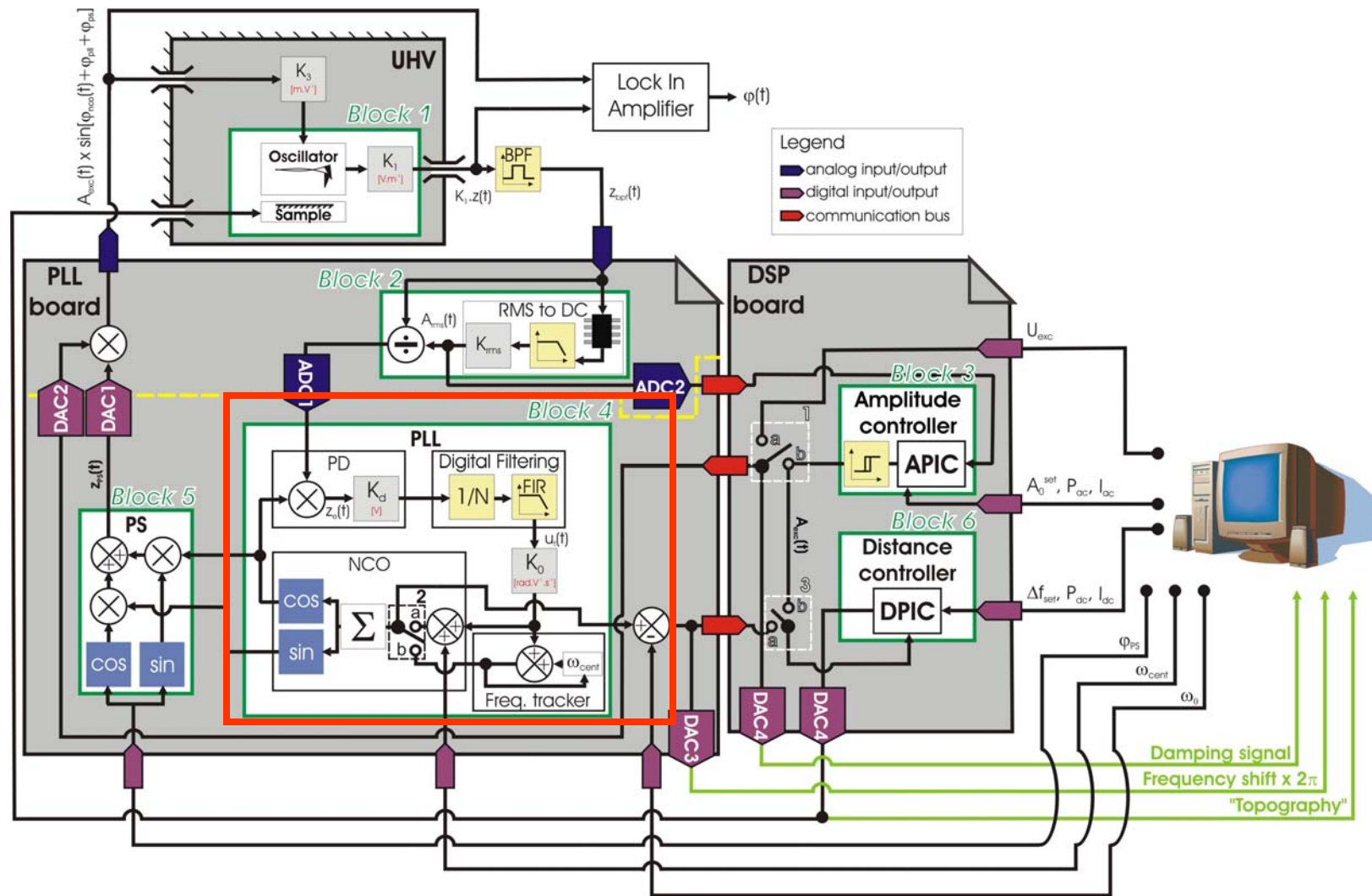
Implementation :

$$D_{amp}(t_i) = P_{ac} [A_0^{set} - A_{rms}(t_i)] + \sum_{j=0}^i I_{ac} [A_0^{set} - A_{rms}(t_j)] \Delta t_b$$

Saturation :  $D_{amp} \in [0; 10V]$

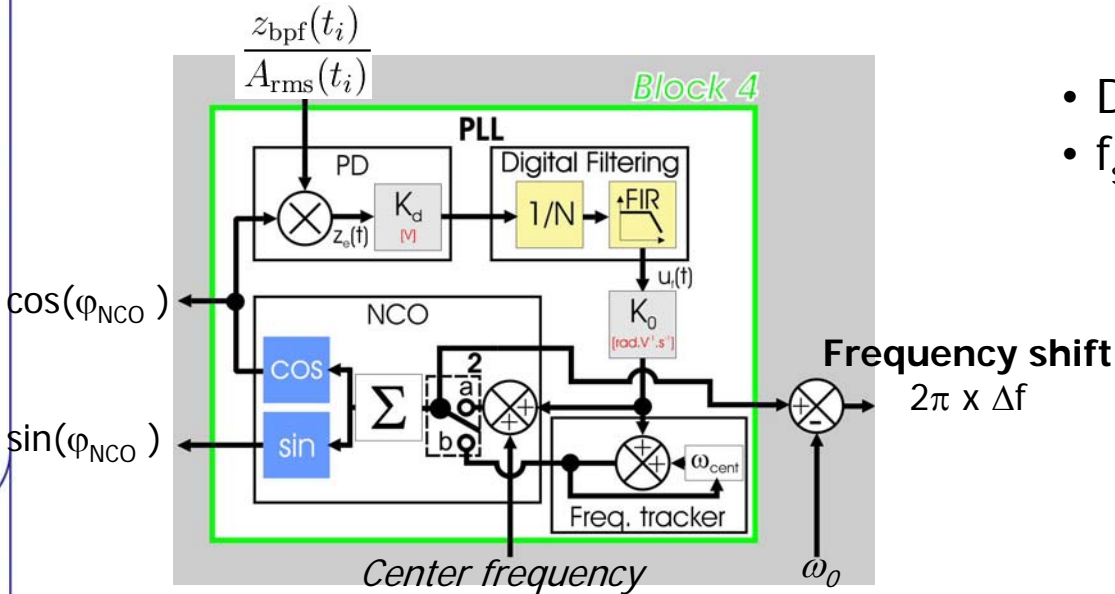


# Block diagram of the electronics





# Block 4, the digital PLL



- Digital device (PLL board)
- $f_s = 20 \text{ MHz}$

Implementation :

$$z_e(t_i) = \frac{z_{bpf}(t_i)}{A_{rms}(t_i)} \times \cos(\varphi_{nco}(t_i))$$

Frequency tracker

Disengaged,  $\omega_{cent} = \text{constant}$

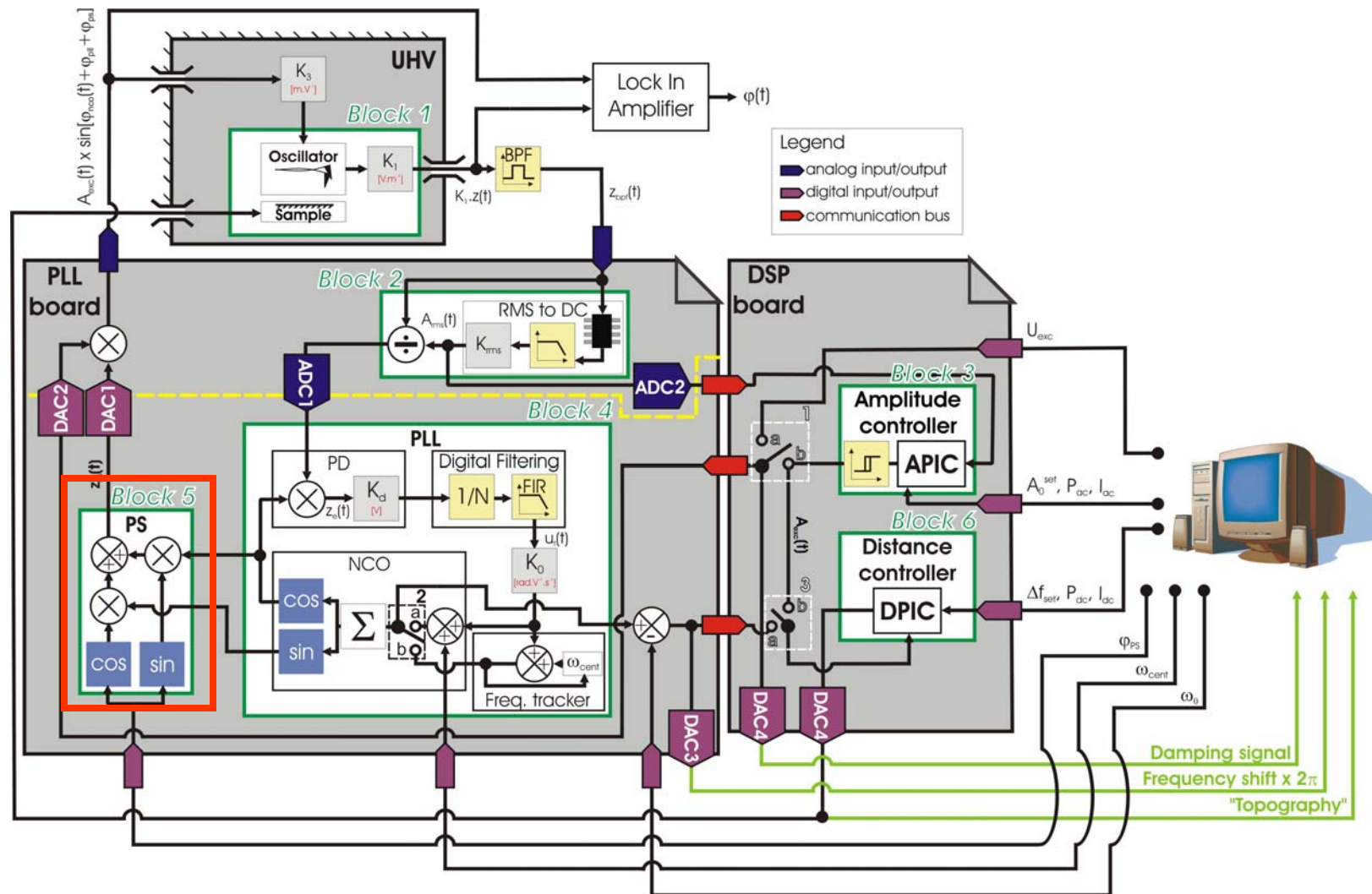
$$\varphi_{nco}(t_i) = \sum_{j=p11}^i [\omega_{cent} + K_0 u_f(t_j)] \Delta t_c$$

Engaged,  $\omega_{cent}$  updated (@ 2.5 kHz)

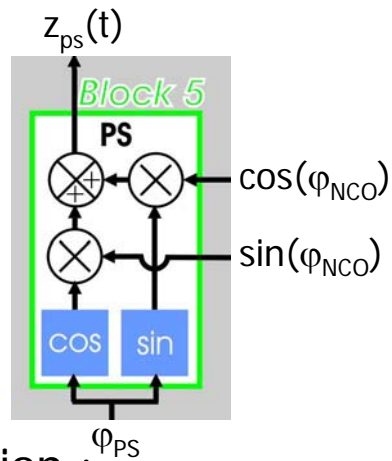
$$\omega_{cent}(t_i) = \omega_{cent}(t_{i-1}) + K_0 \times u_f(t_{i-1})$$

$$\varphi_{nco}(t_i) = \sum_{j=p11}^i \omega_{cent}(t_j) \times \Delta t_c$$

# Block diagram of the electronics



# Block 5, the phase shifter

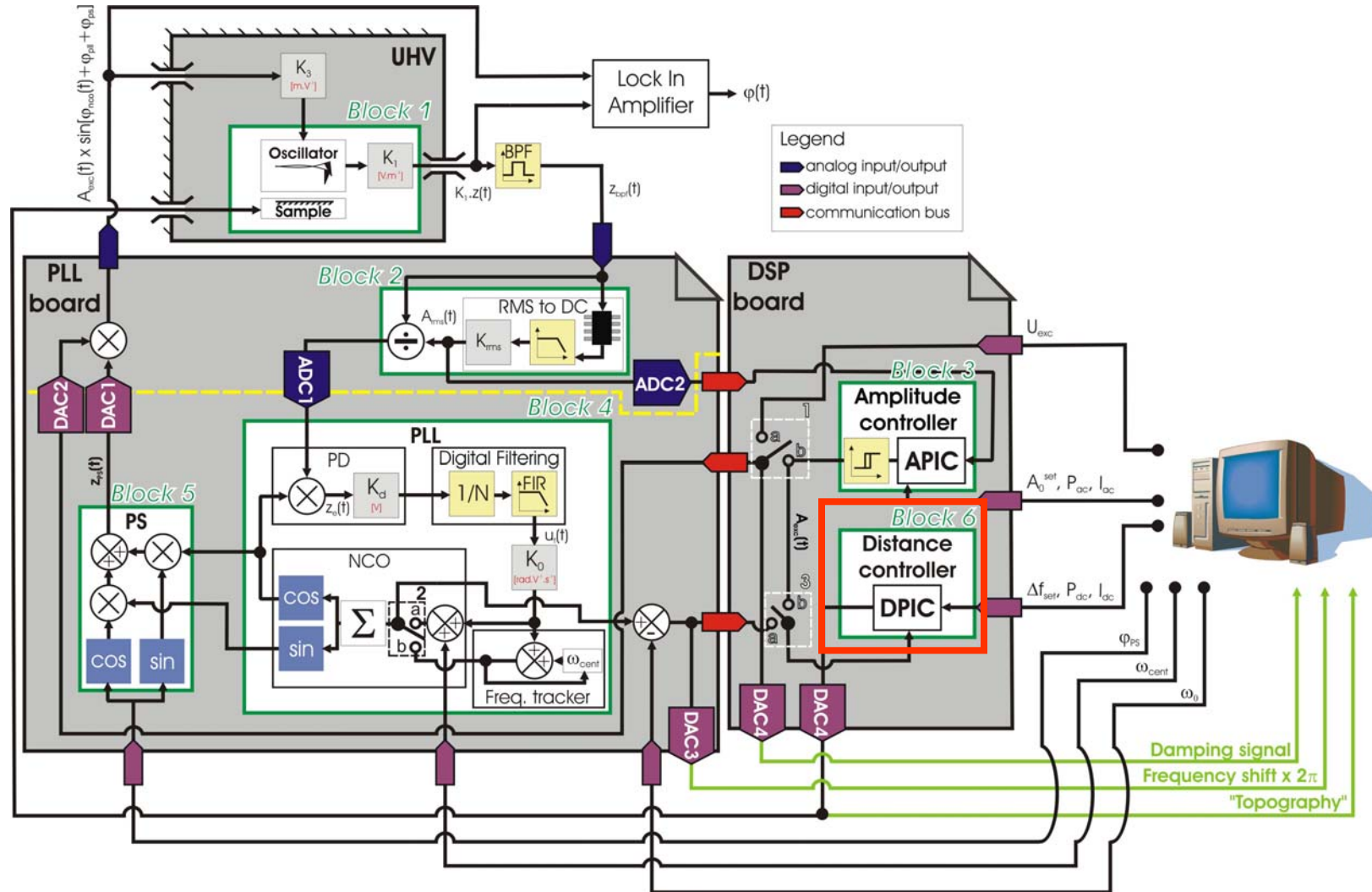


- Digital device (PLL board)
- $f_s = 20 \text{ MHz}$

Implementation :

$$\begin{aligned} z_{ps}(t_i) &= \sin(\varphi_{nco}(t_i)) \times \cos(\varphi_{ps}) + \cos(\varphi_{nco}(t_i)) \times \sin(\varphi_{ps}) \\ &= \sin(\varphi_{nco}(t_i) + \varphi_{ps}) \end{aligned}$$

# Block diagram of the electronics

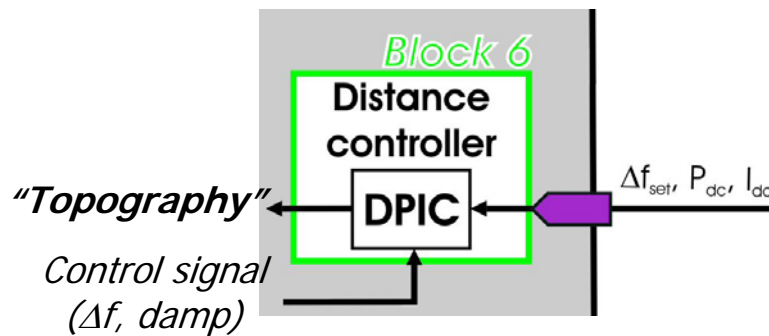


# Block 6, the distance controller (DPIC)

Results

Description

Introduction



- Digital device (DSP board)
- Provides the output signal @  $f_s = 10$  kHz

Implementation :

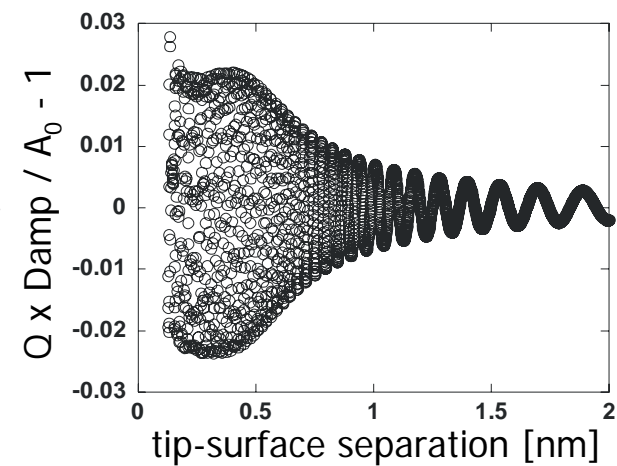
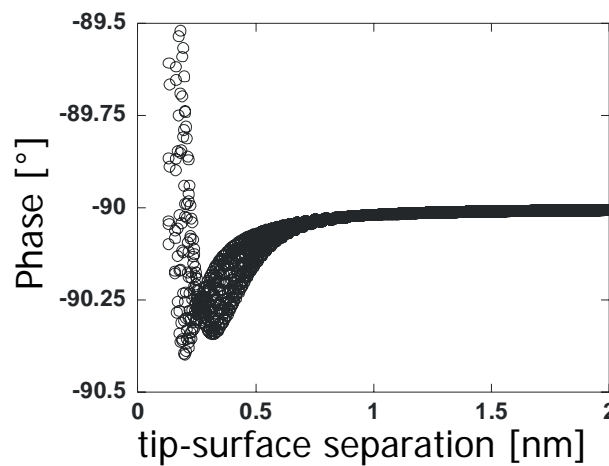
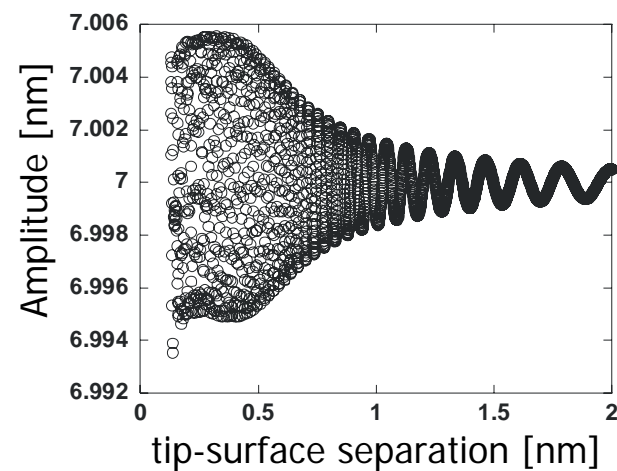
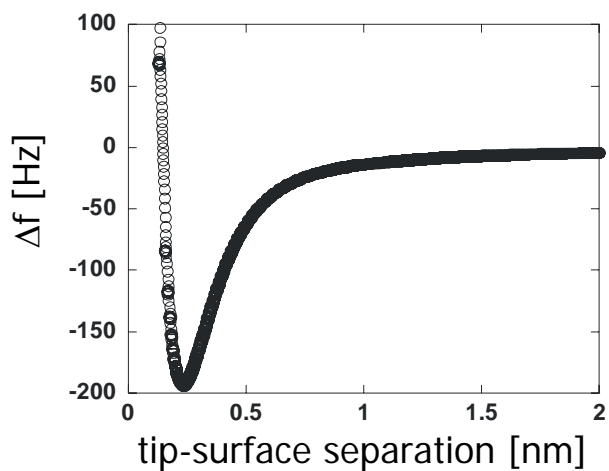
$$D(t_i) = P_{dc} [\Delta f^{\text{set}} - \Delta f(t_i)] + \sum_{j=0}^i I_{dc} [\Delta f^{\text{set}} - \Delta f(t_j)] \Delta t_b$$

# Validation of the virtual setup (1)

Results

Description

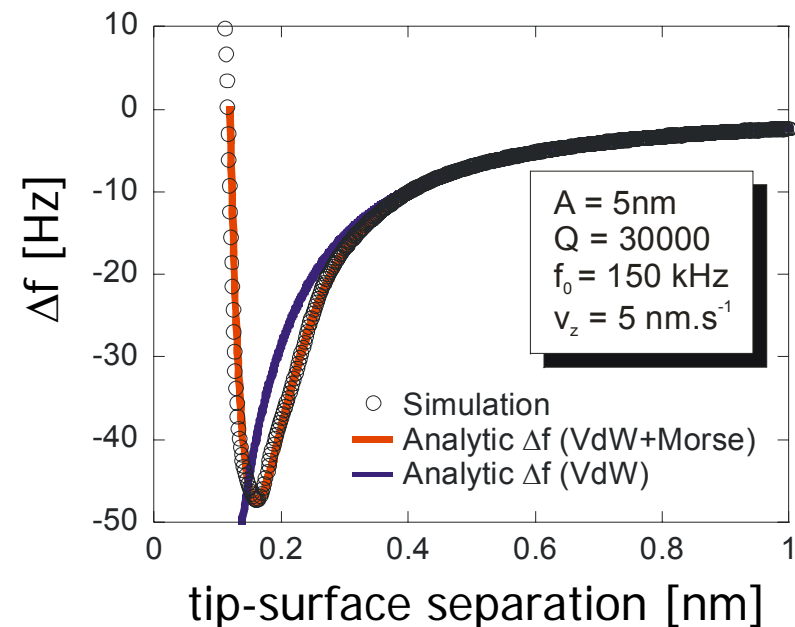
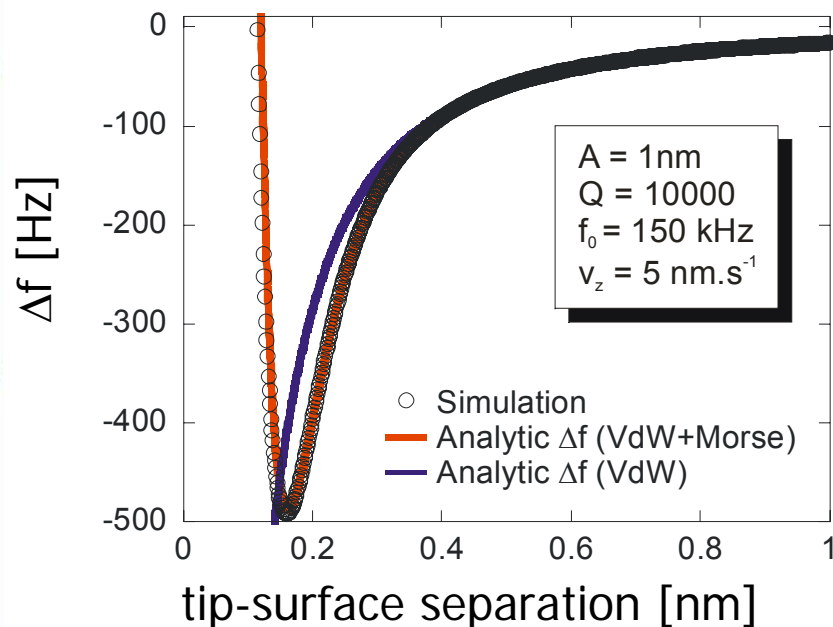
Introduction





## Validation of the virtual setup (2)

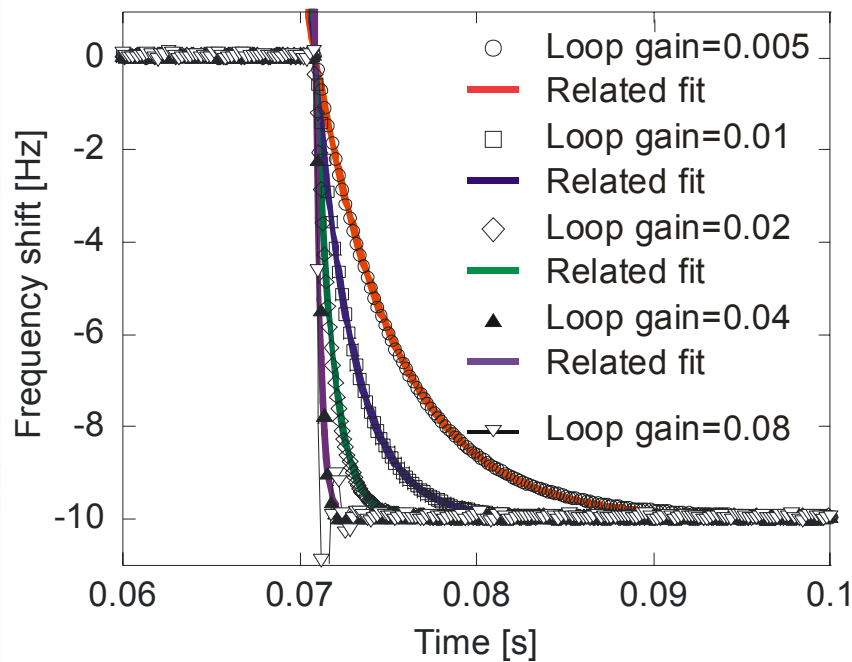
- Comparison with analytic expressions which do not take into account the finite response of the controllers, valid if  $k_c A_0 \gg |F_{int}|$ :



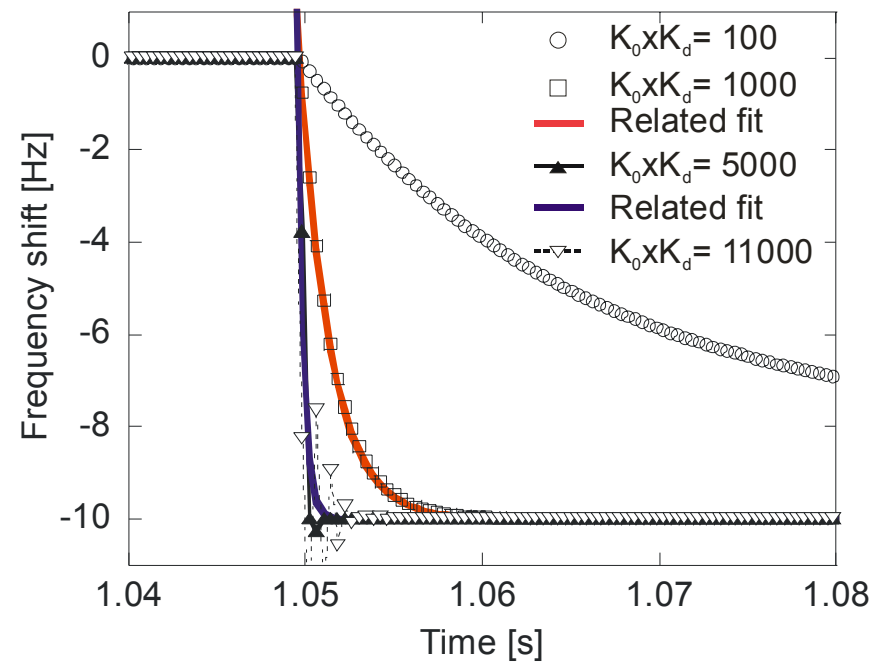
# Dynamic properties of the PLL

- Step response (-10 Hz) analysis and fit with a decaying exponential :

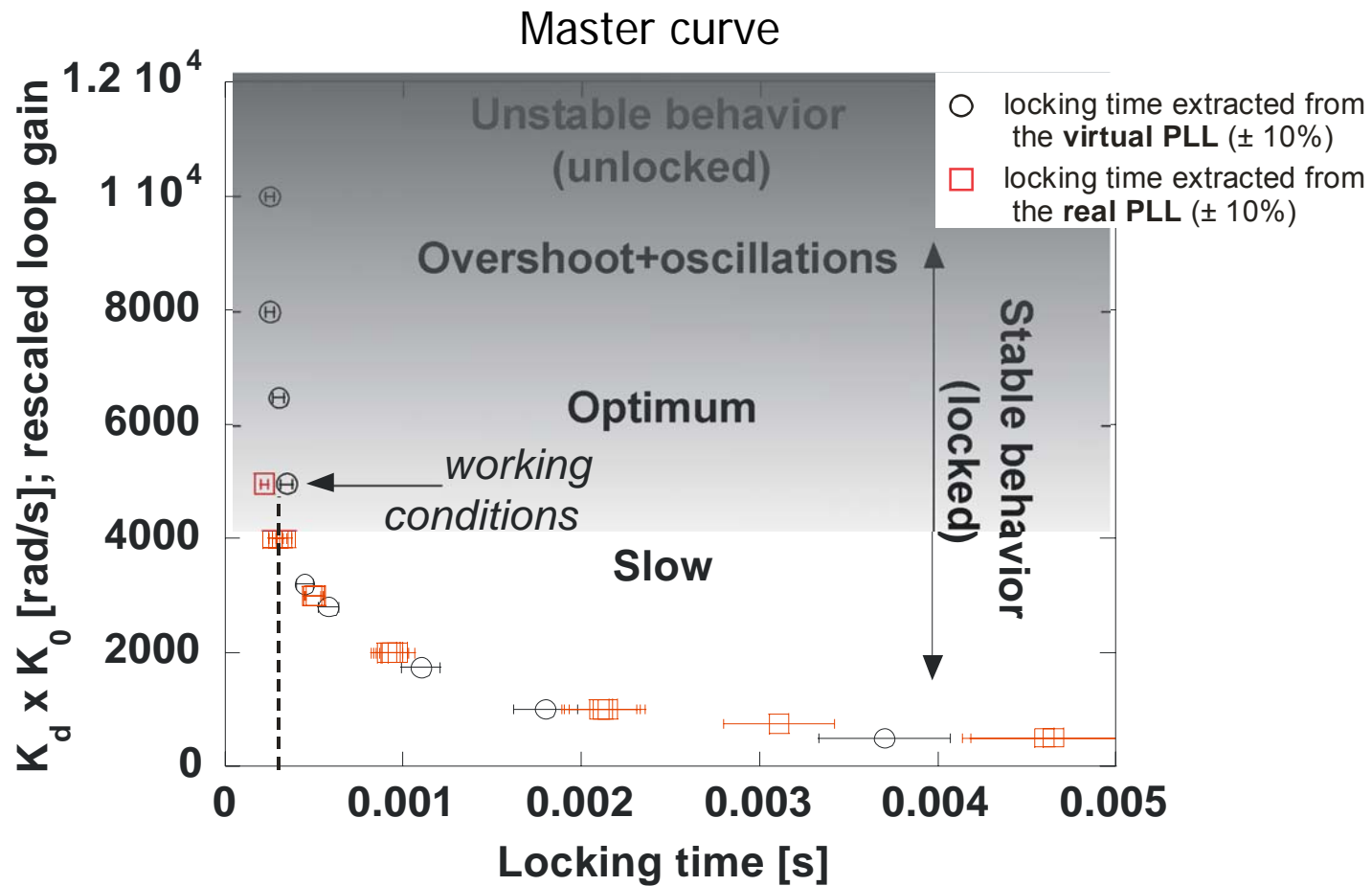
*Real PLL*



*Virtual PLL*



# Dynamic properties of the PLL



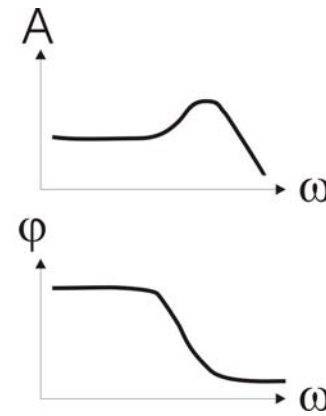
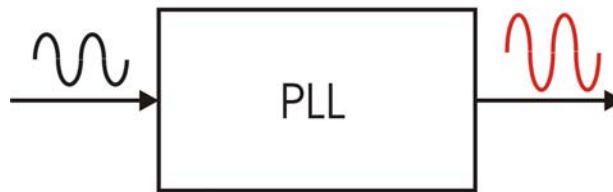
Optimum conditions  $t_{PLL} \sim 0.35$  ms

# The (key) role of the frequency tracker

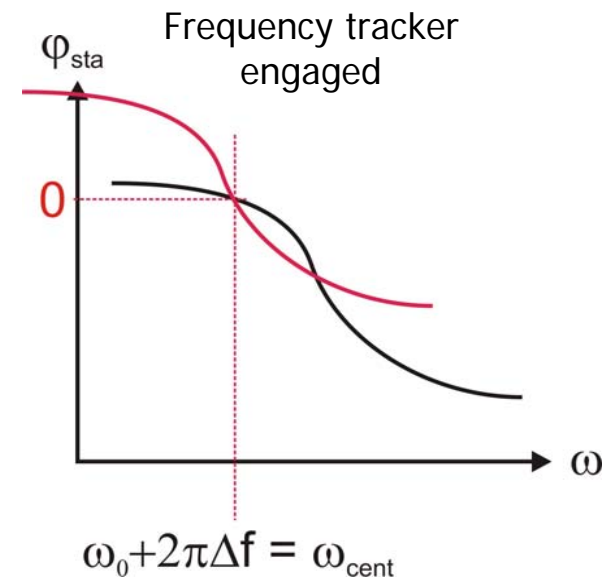
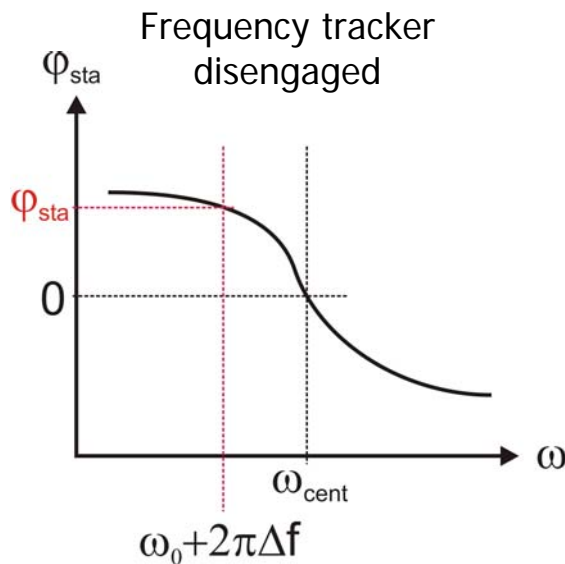
Results

Description

Introduction



Upon approaching the surface, the frequency shifts :



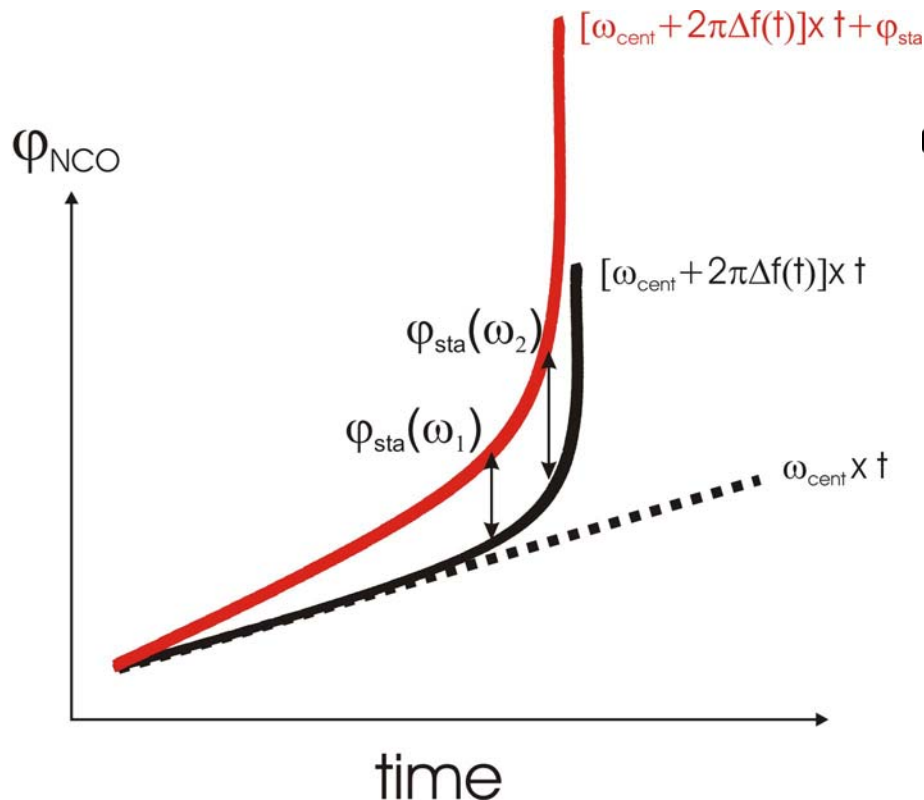
# The (key) role of the frequency tracker

Results

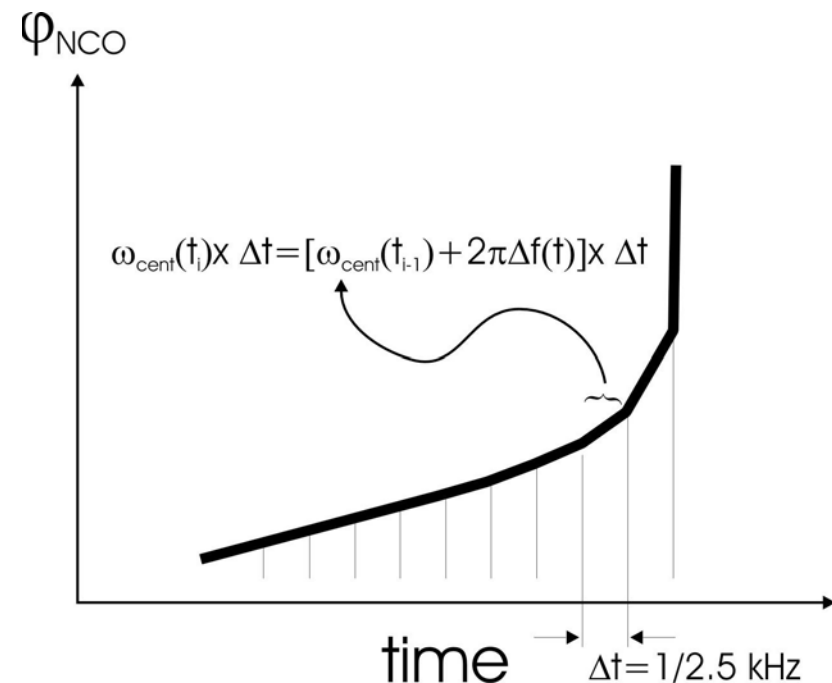
Description

Introduction

Frequency tracker  
disengaged



Frequency tracker  
engaged



With the current design, the PLL locks **the time dependent phase** of the input signal **but can generate an additional static phase lag**



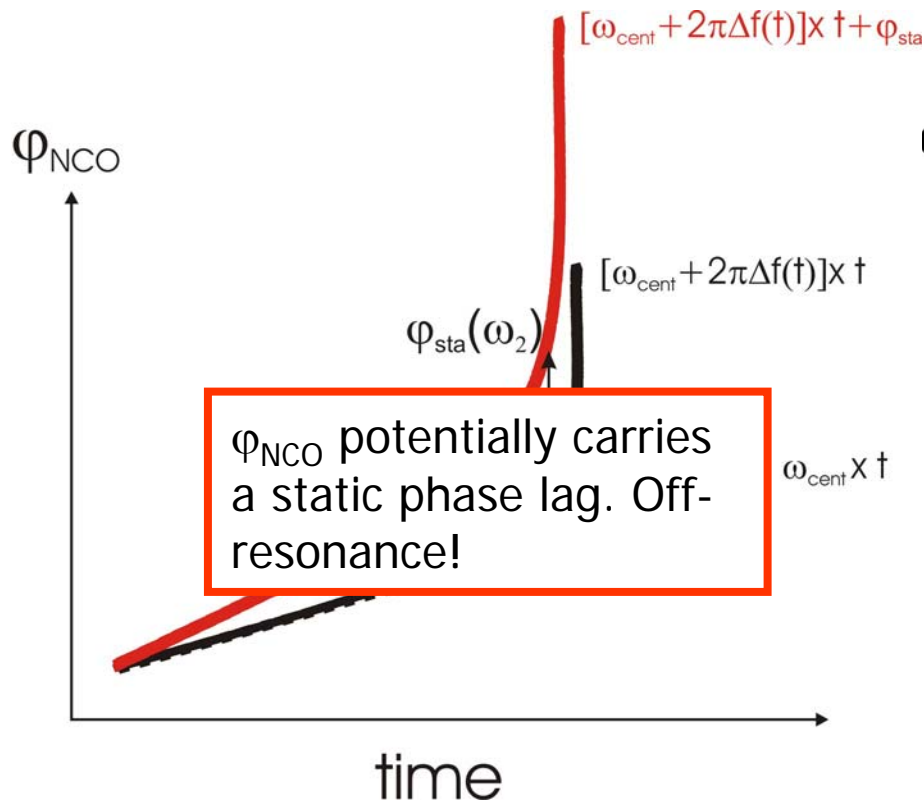
# The (key) role of the frequency tracker

Results

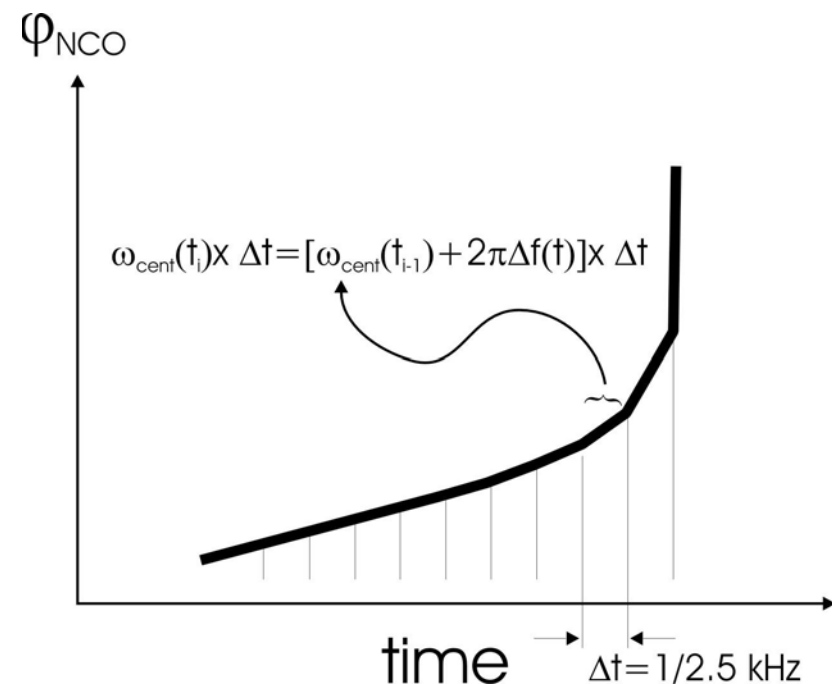
Description

Introduction

Frequency tracker  
disengaged



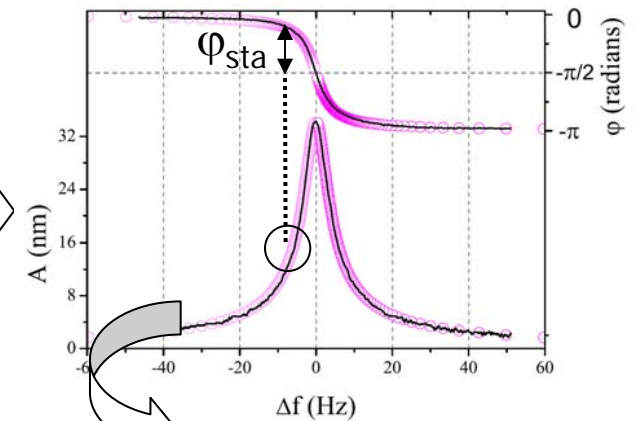
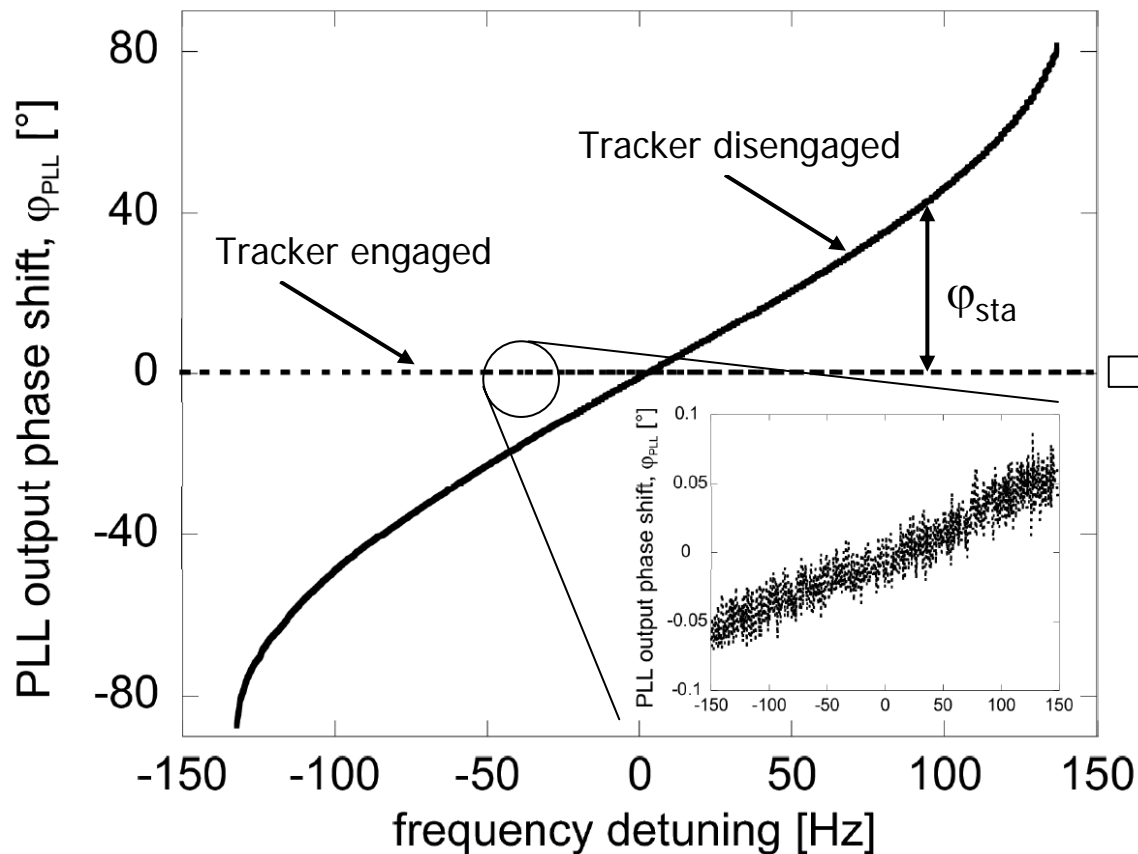
Frequency tracker  
engaged



With the current design, the PLL locks **the time dependent phase** of the input signal **but can generate an additional static phase lag**

# Experimental illustration

The PLL is fed with a 150 kHz sinusoidal waveform, the frequency of which is slowly detuned. The phase shift between input and output is monitored with a lock in amplifier.

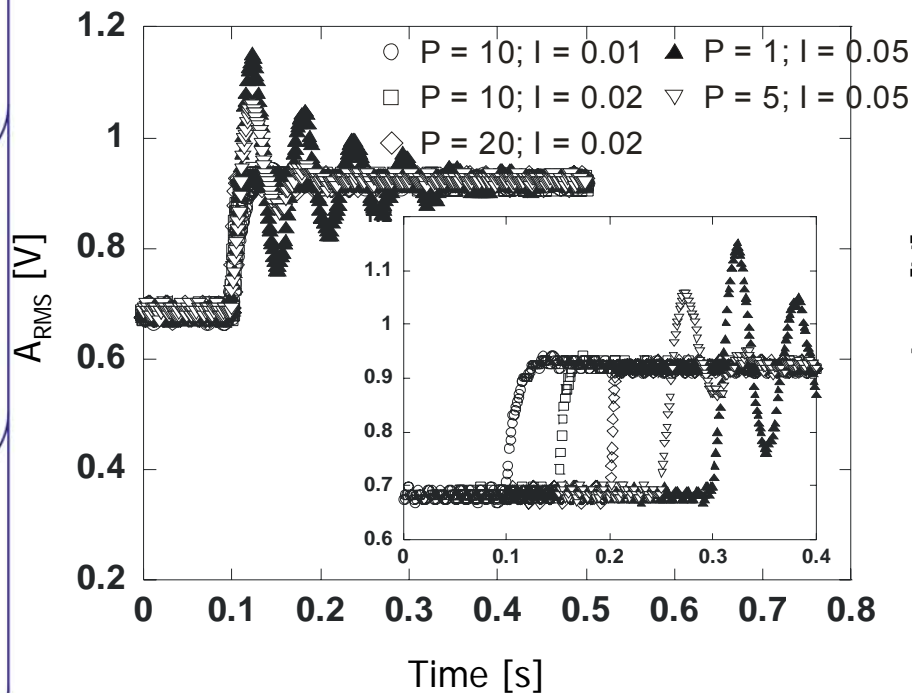


System driven off resonance  
→ **amplitude drops down**  
→ **apparent damping**

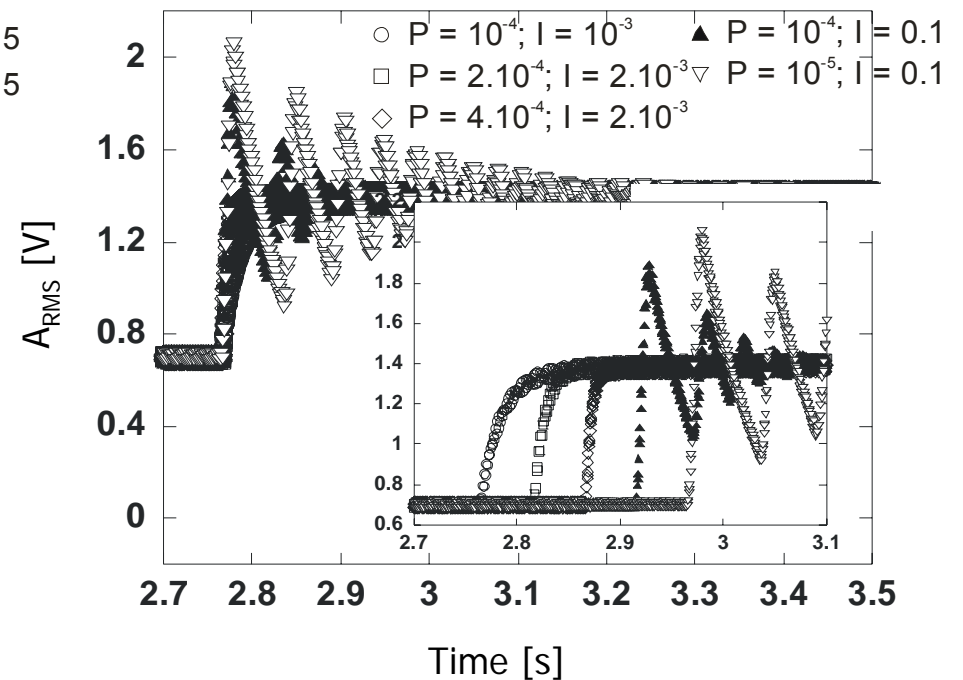
# Dynamic properties of the APIC

- Step response ( $A_{RMS} \times 2$ ) analysis and fit with a decaying exponential for the lone pairs of P,I gains leading to a **critically damped response**:

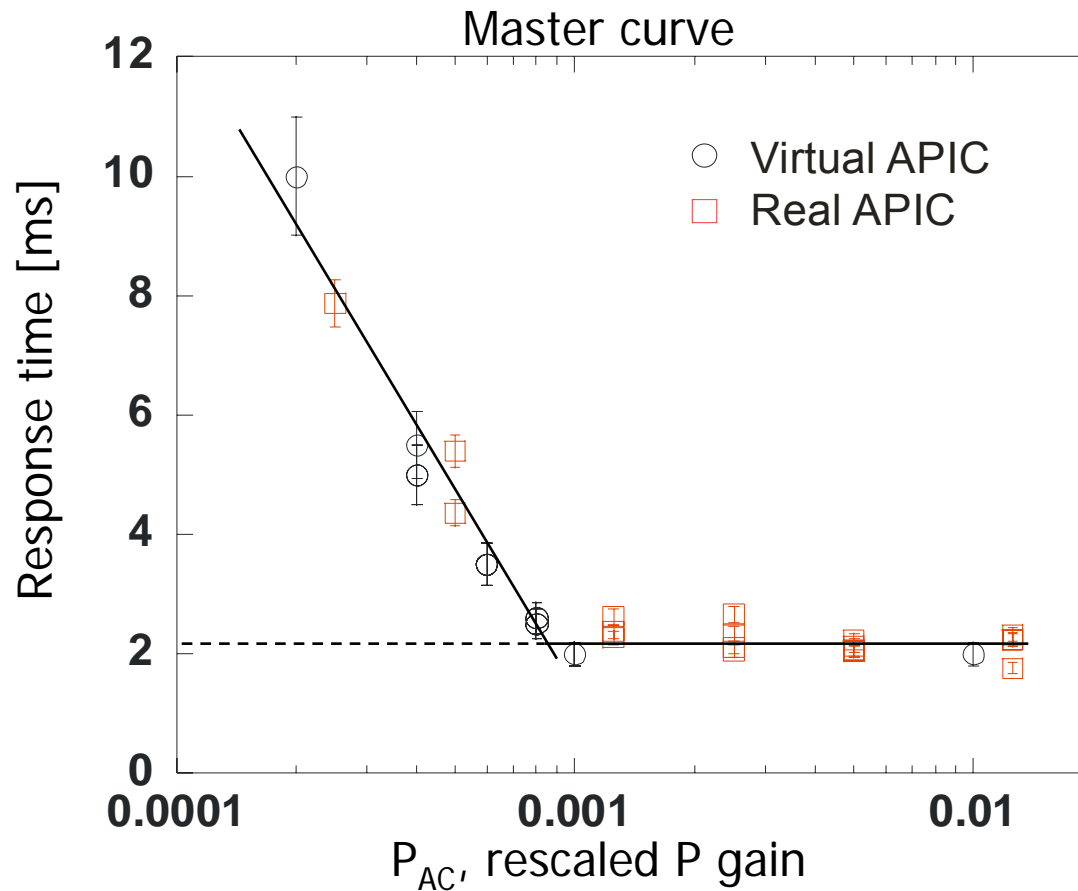
*Real PLL*



*Virtual PLL*



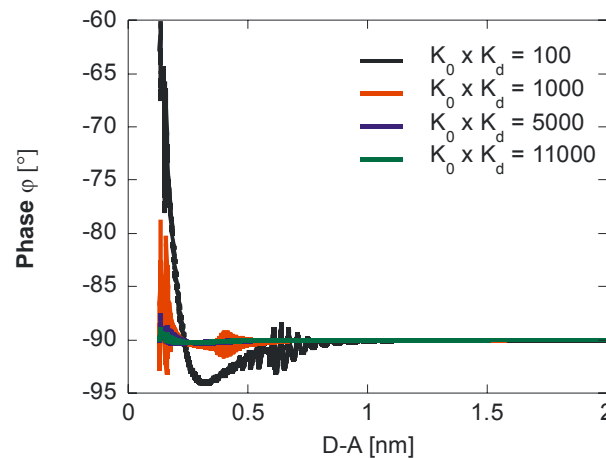
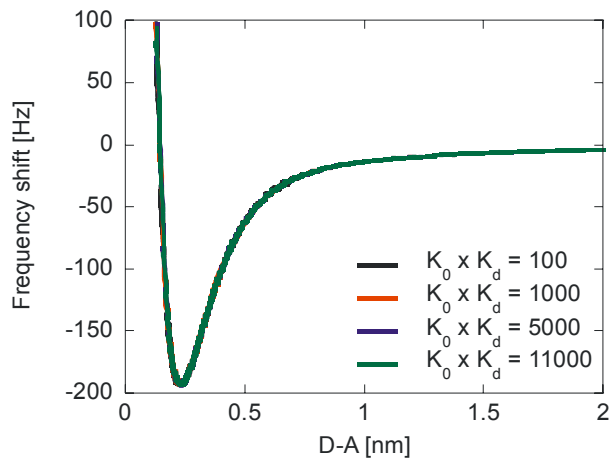
# Dynamic properties of the APIC



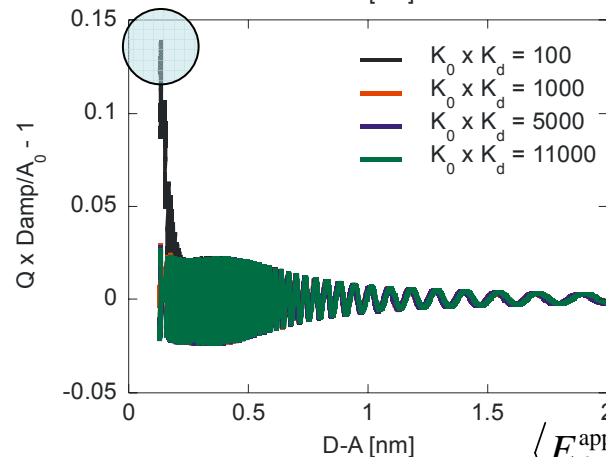
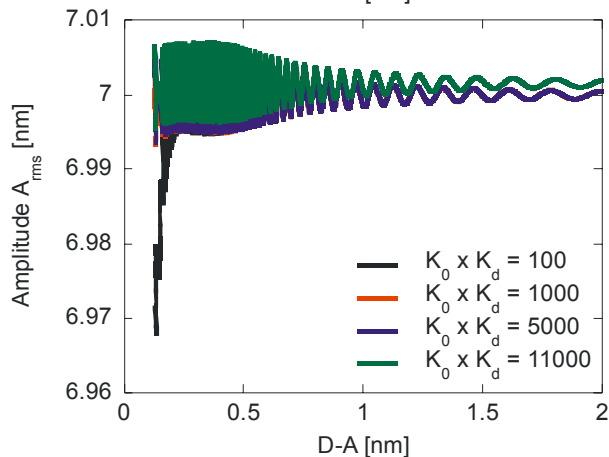
Optimum conditions  $t_{APIC} \sim 2.1$  ms

# Approach curves : apparent damping (1)

- Contribution of the PLL locking time: varying  $K_0 \times K_d$  (frequency tracker engaged)



$K_0 K_d = 100$  ;  $t_{\text{lock}} > 5$  ms  
 $K_0 K_d = 1000$  ;  $t_{\text{lock}} \sim 2$  ms  
 $K_0 K_d = 5000$  ;  $t_{\text{lock}} \sim 0.35$  ms  
 $K_0 K_d = 11000$  ;  $t_{\text{lock}} < 0.2$  ms (nervous)



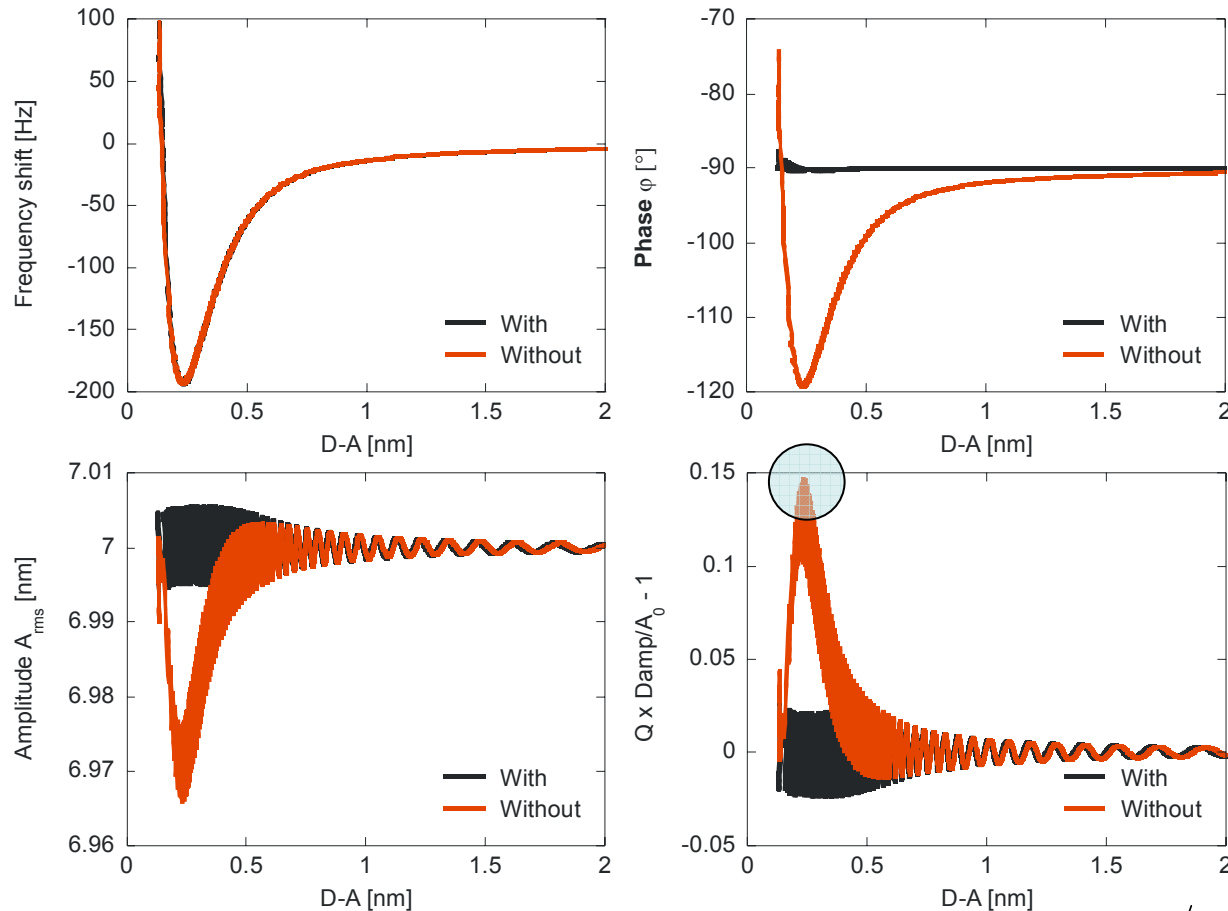
Intrinsic damping :  
 $\langle E_{\text{diss}}^{\text{intr}} \rangle_T = 2 \text{ eV/cycle}$

Apparent damping :  
 $\langle E_{\text{diss}}^{\text{app}} \rangle_T = 14\% \langle E_{\text{diss}}^{\text{intr}} \rangle_T \cong 0.28 \text{ eV/cycle}$



# Approach curves : apparent damping (2)

- Contribution of the frequency tracker



Apparent damping :

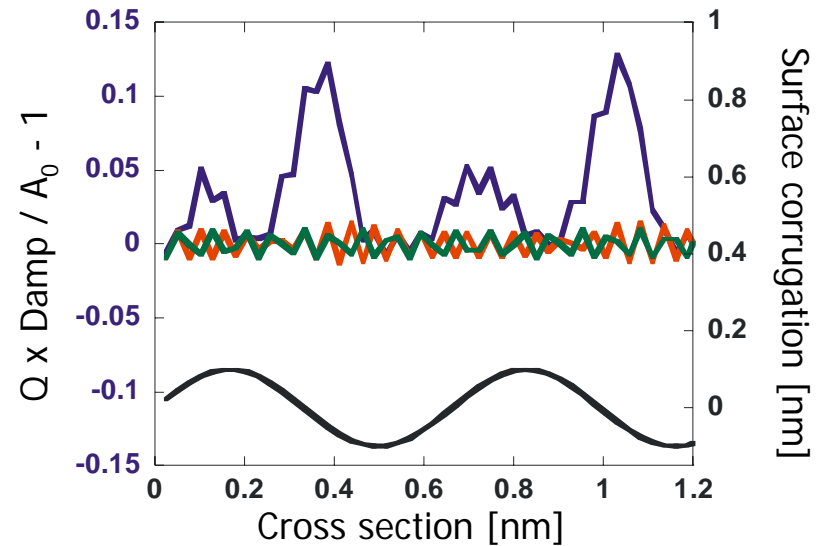
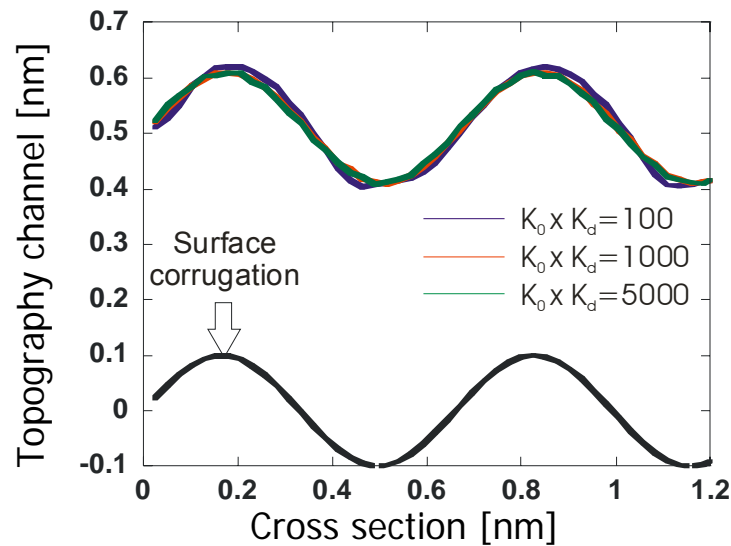
$$\langle E_{diss}^{app} \rangle_T = 14\% \langle E_{diss}^{intr} \rangle_T \cong 0.28 \text{ eV/cycle}$$

# Summary

- **PLL dynamics** : **major role** in the occurrence of relevant **apparent damping** if the **locking time is about or larger than 1~ms**, that is only twice faster than the APIC optimum response time
- The **frequency tracker**, the aim of which is to update the PLL center frequency to make it matching the actual resonance frequency, plays also a **major role** in the occurrence of **apparent damping**. It has to be engaged when performing approach curves
- The **PLL optimal locking time is about 0.35 ms that is 6 times shorter than the shortest APIC response time** of the free cantilever. Therefore **the resonance condition is expected to be always properly maintained**. Consequently, when the PLL operates properly, **no amplitude changes due to a bad tracking of the resonance frequency are expected to occur**
- The APIC response time seems to be limited to ~2 ms due to the RMS-to-DC converter

# Scan lines ( $\Delta f$ regulation) (1)

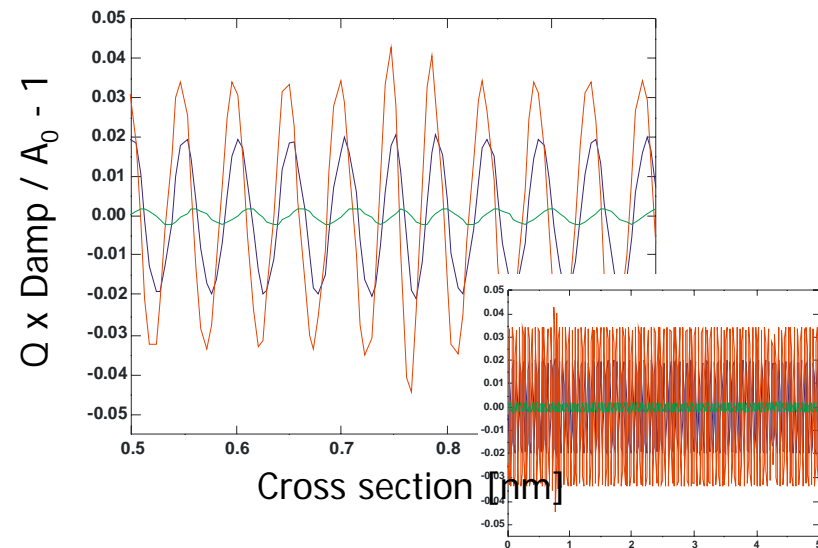
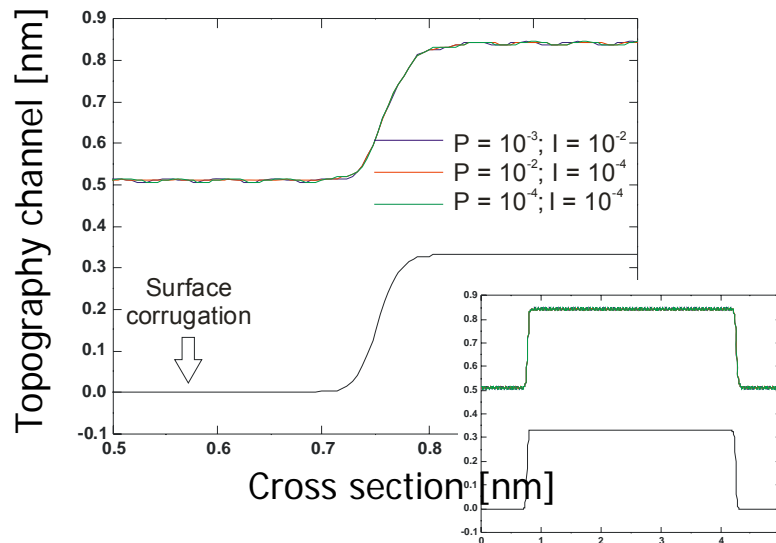
- Contribution of the PLL
  - Sinusoidally corrugated surface ( $\lambda = 6.6 \text{ \AA}$ )
  - 256 points per line
  - $v_x = 7 \text{ nm.s}^{-1}$ ,  $P_{AC} = 10^{-3}$ ,  $I_{AC} = 10^{-4} \text{ s}^{-1}$
  - Frequency tracker engaged



➔ { Negligible effect on the topography  
Negligible apparent damping except if PLL is slow

# Scan lines ( $\Delta f$ regulation) (2)

- Contribution of the APIC
  - Surface with opposite steps (height : 3.3 Å)
  - 1024 points per line
  - $v_x = 5 \text{ nm.s}^{-1}$ ,  $K_0 \times K_d = 5000 \text{ rad.s}^{-1}$
  - Frequency tracker engaged



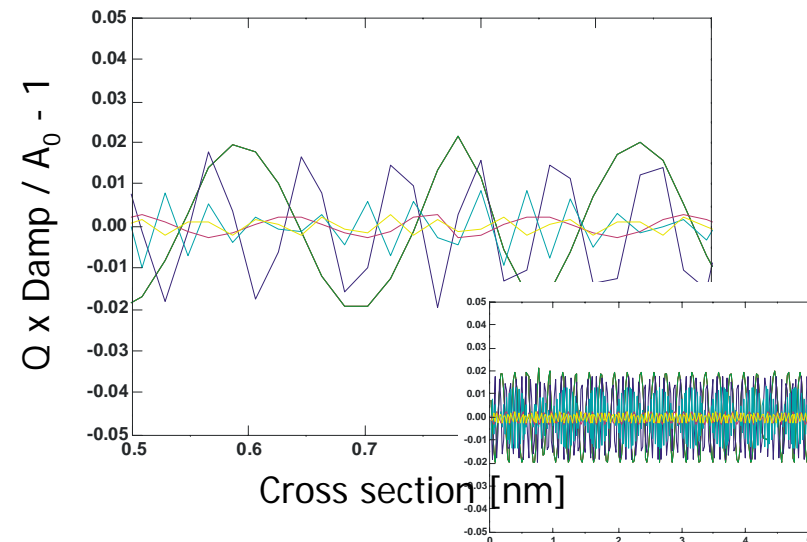
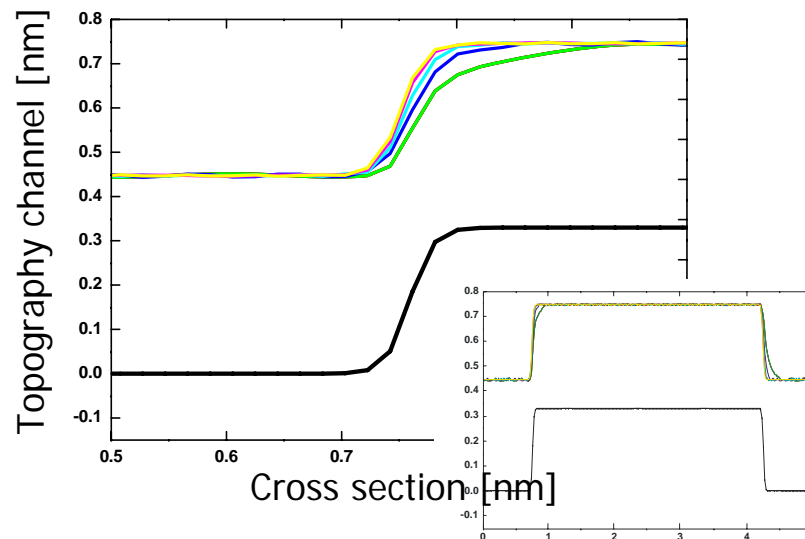
➔ Negligible effect on the topography  
Weak apparent damping (not experimentally relevant) provided APIC is fast

# Scan lines ( $\Delta f$ regulation) (3)

- Contribution of the scanning speed

- Surface with opposite steps (height : 3.3 Å)
- 256 points per line
- $P_{AC}=10^{-3}$ ,  $I_{AC}=10^{-4} \text{ s}^{-1}$ ,  $K_0 \times K_d = 5000 \text{ rad.s}^{-1}$
- Frequency tracker engaged

- 1 nm/s
- 2 nm/s
- 5 nm/s
- 10 nm/s
- 20 nm/s



➔ { Distorted topography at high  $v_x$   
Weak apparent damping (not experimentally relevant)

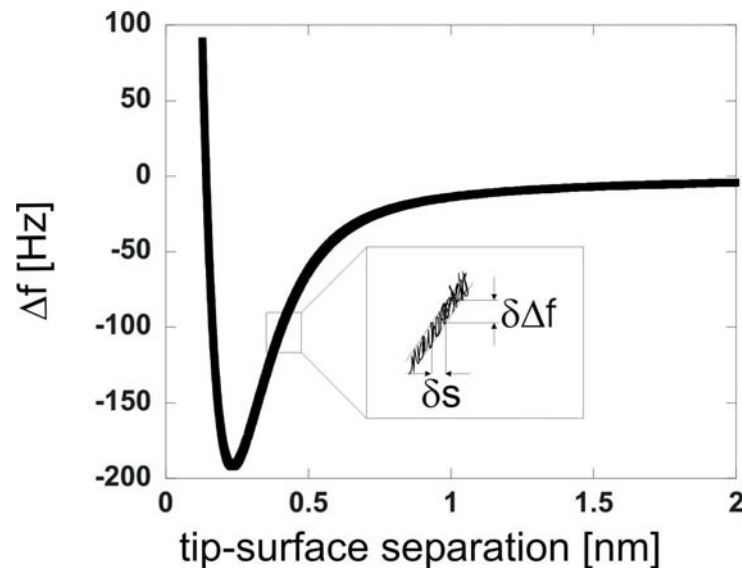


# Summary

- PLL dynamics : major role in the occurrence of relevant apparent damping if the locking time is about or larger than 1~ms, that is only twice faster than the APIC optimum response time
- The frequency tracker, the aim of which is to update the PLL center frequency to make it matching the actual resonance frequency, plays also a major role in the occurrence of apparent damping. It has to be engaged when performing approach curves
- The PLL optimal locking time is about 0.35 ms that is 6 times shorter than the shortest APIC response time of the free cantilever. Therefore the resonance condition is expected to be always properly maintained. Consequently, when the PLL operates properly, no amplitude changes due to a bad tracking of the resonance frequency are expected to occur
- The APIC response time seems to be limited to ~2 ms due to the RMS-to-DC converter
- **A weak contribution of the APIC to apparent dissipation is observed.** Although spatial shift and apparent dissipation can conditionally be generated, the overall strength of the effect remains weak and should hardly be measurable for UHV investigations at room temperature.

# Is the apparent damping relevant?

Simplest assumption: what is the dissipated energy of the cantilever due to thermal fluctuations when oscillating close to the surface?



$$k_B T \Rightarrow \delta A_0 (\delta s) \Rightarrow \delta F_{\text{int}} (\delta \Delta f) \Rightarrow \delta A_{\text{exc}}$$

To first order:

$$\frac{\delta A_{\text{exc}}}{A_0} = \frac{\delta F_{\text{int}}}{k_c A_0} \Rightarrow \delta E_d = \pi A_0 \delta F_{\text{int}}$$

$\Delta f$  is connected to  $F_{\text{int}}$  [1]:

$$\frac{\Delta f k_c A_0^{3/2}}{f_0} \simeq 0.43 \sqrt{V_{\text{int}}(r) F_{\text{int}}(r)} \Rightarrow \frac{\delta f}{f_0} \simeq \frac{0.43}{2k_c A_0^{3/2}} \sqrt{\frac{V_{\text{int}}(r)}{F_{\text{int}}(r)}} \delta F_{\text{int}}$$

The frequency noise is given by [2]:

$$\frac{\delta f}{f_0} = \sqrt{\frac{2k_B T B}{\pi^3 k_c A_0^2 f_0 Q}} \Rightarrow \delta E_d \simeq 4.6 \sqrt{\frac{2k_B T B k_c A_0^3 F_{\text{int}}(r)}{\pi f_0 Q V_{\text{int}}(r)}}$$

[1]- H.-J. Ke *et al.*, **Noncontact Atomic Force Microscopy**, Eds Morita, Wiesendanger, Meyer, Springer Berlin, Germany 2002

[2]- F.J. Giessibl, ch2 in ref.[1]

# Is the apparent damping relevant?

Parameters :  $A_0=7\text{nm}$ ,  $f_0=150\text{ kHz}$ ,  $k_c=40\text{ Nm}^{-1}$ ,  $B=260\text{ Hz}$   
interaction parameters taken from [1] at  $s=5\text{ \AA}$

$Q$	$E_0$ (eV/cycle)	$\delta E_d$ (eV/cycle)	$\delta E_d/E_0$	$\delta E_d$ (eV/cycle)	$\delta E_d/E_0$
	VdW + short range			Pure VdW	
5000 ( $T = 298^\circ\text{K}$ )	7.69	0.177	2.30%	0.141	1.84%
30000 ( $T = 298^\circ\text{K}$ )	1.28	$7.25 \times 10^{-2}$	5.65%	$5.78 \times 10^{-2}$	4.50%
500000 ( $T = 4^\circ\text{K}$ )	0.077	$2.06 \times 10^{-3}$	2.67%	$1.64 \times 10^{-3}$	2.13%

- Apparent dissipation due to PLL would be detected if it would occur (15%)
- Gauthier *et al.* put in evidence effects that are in the 5% range, not relevant in UHV at room temperature! With the conditions given in his work:

$$\delta E_d/E_0 \sim 27\%$$

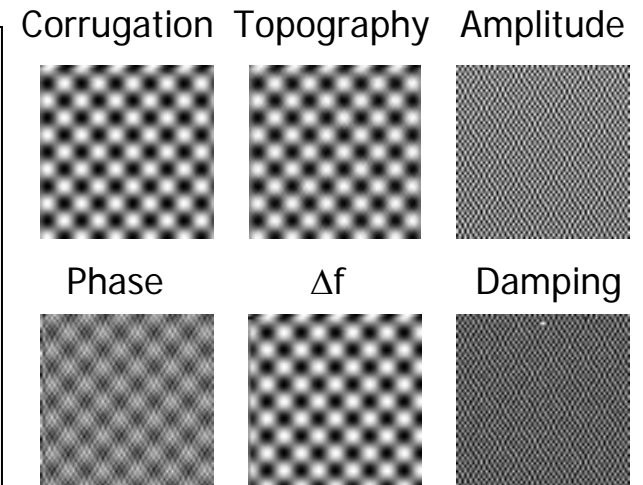
Does not explain the shift but dissipation observed at steps is likely real dissipation

[1]- R. Pérez *et al.*, Phys. Rev. B **58**, 10835 (1998)

# Summary and Outlooks

- ✓ Implementation of the real setup
- ✓ Reasonable description of the dynamic properties of the PLL (amplitude controller as well)
- ✓ Relevant apparent dissipation can conditionally be observed (PLL gains and frequency tracker)

- ☐ Investigation of the stability
- ☐ Contribution of noise
- ☐ Realistic force fields (SciFi)
- ☐ Atomistic description of damping
- ☐ Calculation of images

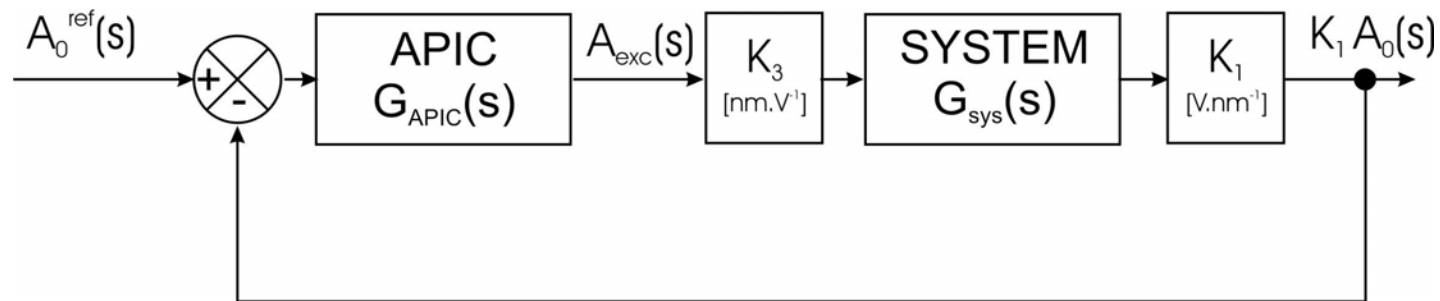


# Questions / Discussions



# Dynamic properties of the APIC

Behavior of the APIC in the closed loop:



- Steady equation of the oscillator amplitude ( $\varphi = -\pi/2$ ,  $\omega = \omega_0$ ) :

$$G_{sys}(s) = \frac{K_1 A_0(s)}{A_{exc}(s)} = \frac{b}{s + a} \quad \left\{ \begin{array}{l} b = \frac{K_1 K_3 \omega_0}{2} \\ a = \frac{\omega_0}{2Q} \end{array} \right.$$

- P, I controller :

$$G_{APIC}(s) = K_P + \frac{K_I}{s}$$

$$\Rightarrow G_{cl}(s) = \frac{K_1 A_0(s)}{A_0^{ref}(s)} = \frac{G_{APIC}(s) G_{sys}(s)}{1 + G_{APIC}(s) G_{sys}(s)}$$

# Dynamic properties of the APIC

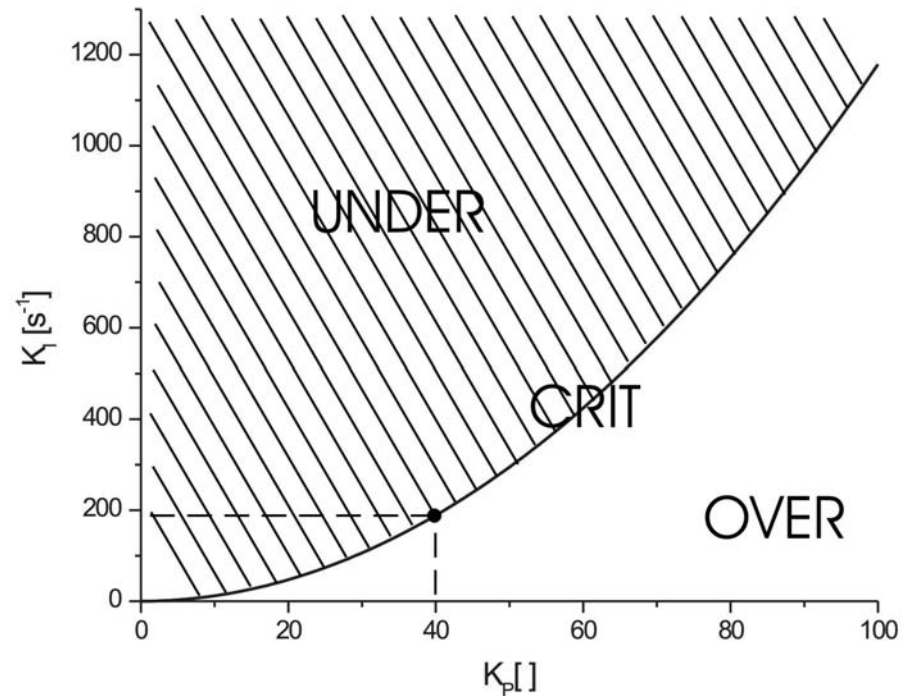
The closed looped system is analogous to a second order system

$$\begin{cases} \text{Undercritically damped regime} \Rightarrow \zeta < 1 \Leftrightarrow c < \sqrt{bK_I} \\ \text{Critically damped regime} \Rightarrow \zeta = 1 \Leftrightarrow c = \sqrt{bK_I} \\ \text{Overcritically damped regime} \Rightarrow \zeta > 1 \Leftrightarrow c > \sqrt{bK_I} \end{cases} \quad c = \frac{a+bK_P}{2}$$

$$K_I = \frac{\omega_0}{8} \left( \frac{1}{Q} + K_1 K_3 K_P \right)^2$$



time constant  
of the system?



# Dynamic properties of the APIC

Analysis of the system response to a step :

$$\mathcal{L}^{-1} \curvearrowright G_s(s) = \frac{A_s}{s}$$

- Overcritically damped regime :

$$g_{cls}(t) = A_s \left\{ 1 + \frac{c-\xi-bK_P}{2\xi} e^{-\underbrace{(c+\xi)t}_{\text{Short time scales}}} - \frac{c+\xi-bK_P}{2\xi} e^{-(c-\xi)t} \right\} \quad \xi = \sqrt{c^2 - bK_I}$$

- Critically damped regime :

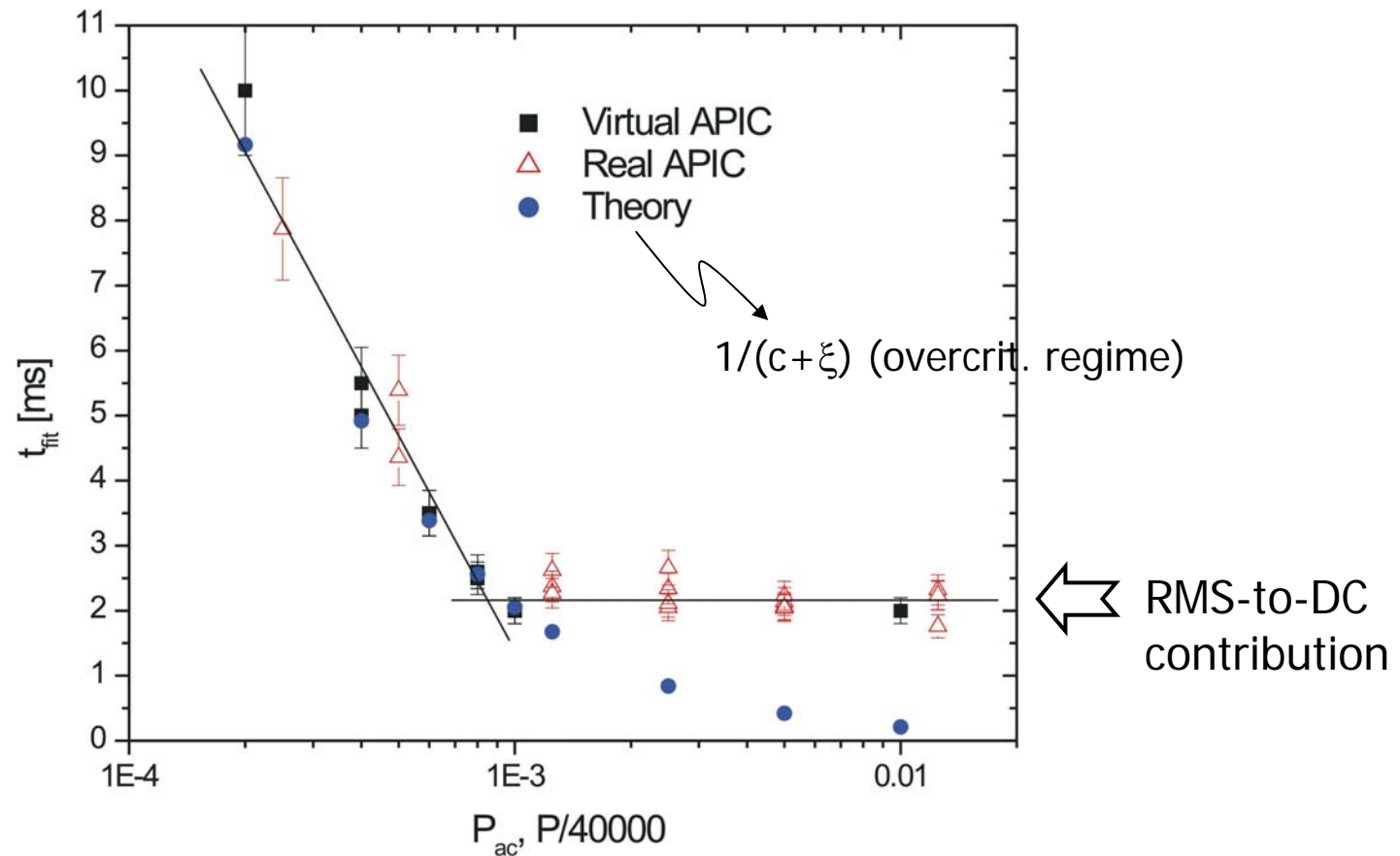
$$g_{cls}(t) = A_s \{ 1 - e^{-ct} + [bK_P - c] t e^{-ct} \}$$

- Undercritically damped regime :

$$g_{cls}(t) = A_s \left\{ 1 - e^{-ct} \times \left[ \cos(\xi' t) + \frac{c-bK_P}{\xi'} \sin(\xi' t) \right] \right\} \quad \xi' = \sqrt{bK_I - c^2}$$

# Dynamic properties of the APIC

Summary :

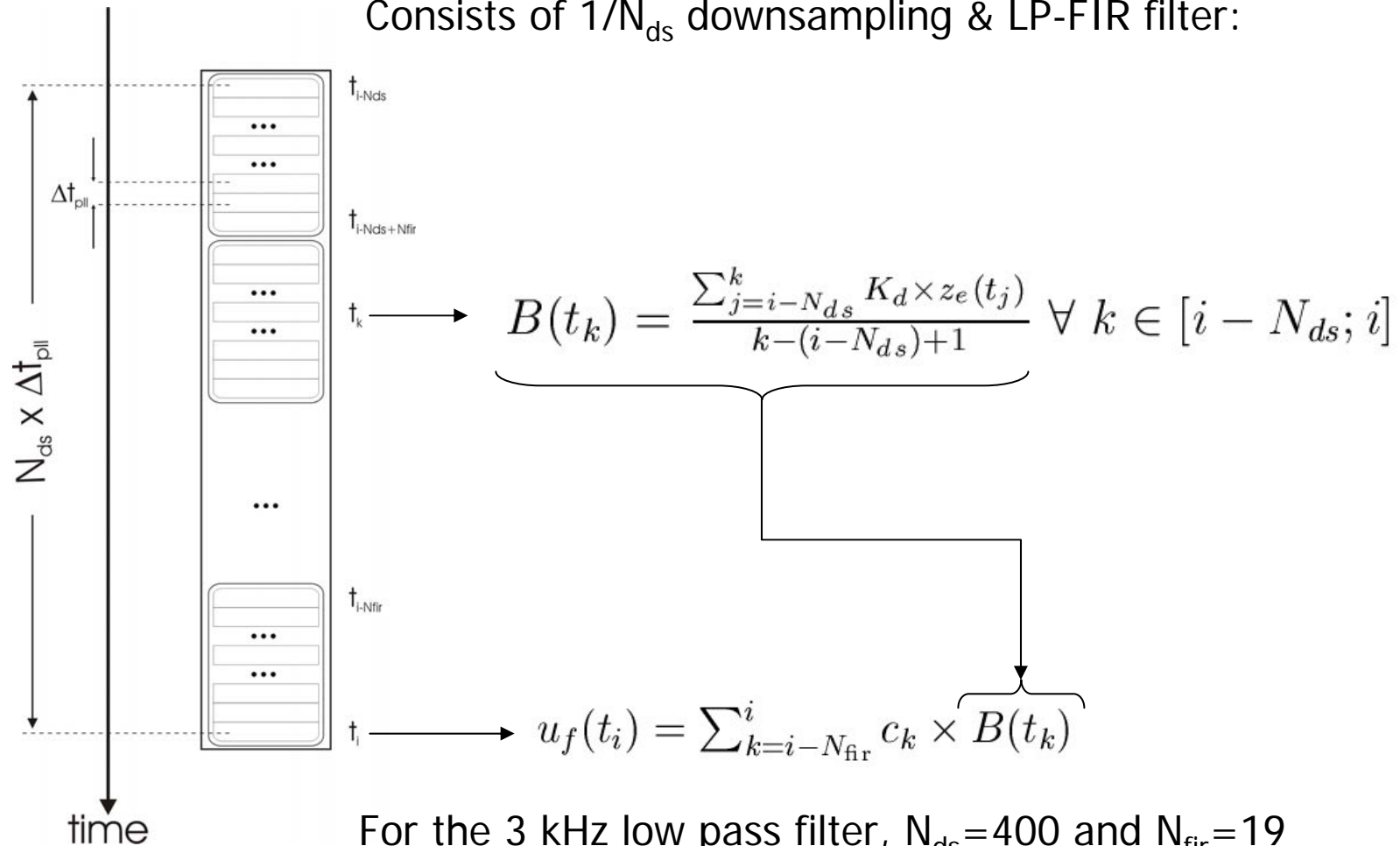


## Remarks

- Time of calculation on a AMD 1700+, 512 Mb RAM
  - Approach curve: 15 nm vertical extension @ 2 nm.s<sup>-1</sup> ~ 45 min.
  - 1 scan line: 7 nm @ 5nm.s<sup>-1</sup> ~ 20 min.

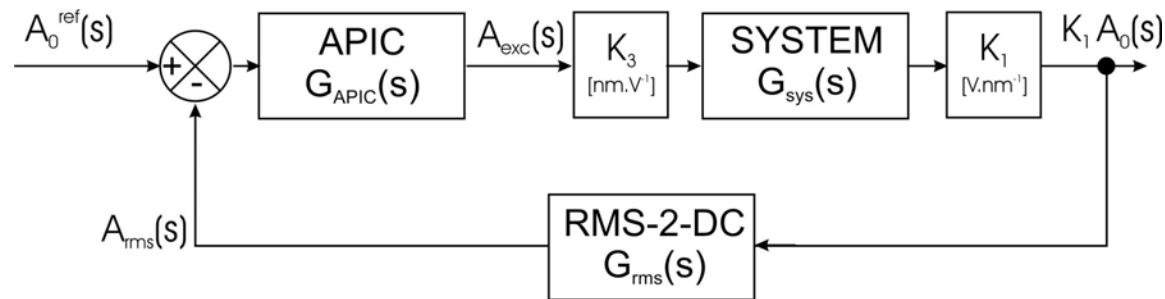
# The digital filtering

Consists of  $1/N_{ds}$  downsampling & LP-FIR filter:





# Stability analysis of the linear closed looped system



1<sup>st</sup> order steady equations

$$\begin{cases} \ddot{A}(t) = A(t) [\omega + \dot{\varphi}(t)]^2 - A(t)\omega_0^2 + K_3 A_{exc}(t)\omega_0^2 \cos(\varphi(t)) - \frac{\omega_0}{Q} \dot{A}(t) \\ \ddot{\varphi}(t) = -\frac{2\dot{A}(t)}{A(t)} [\omega + \dot{\varphi}(t)] - \frac{K_3 A_{exc}(t)\omega_0^2}{A(t)} \sin(\varphi(t)) - \frac{\omega_0}{Q} [\omega + \dot{\varphi}(t)] \\ K_3 \dot{A}_{exc}(t) = -K_1 K_3 K_P d A(t) + K_3 K_P d A_{rms}(t) + K_3 K_I [A_0^{ref} - A_{rms}(t)] \\ \frac{\dot{A}_{rms}(t)}{K_1} = d A(t) - d \frac{A_{rms}(t)}{K_1} \end{cases}$$

$$\begin{pmatrix} \dot{\Lambda} \\ \dot{P} \\ \Lambda \\ P \\ K_3 \dot{x} \\ \dot{r}/K_1 \end{pmatrix} = M \begin{pmatrix} \dot{\alpha} \\ \dot{p} \\ \alpha \\ p \\ K_3 x \\ r/K_1 \end{pmatrix} \quad \text{with} \quad M = \begin{pmatrix} -\frac{\omega_0}{Q} & 2\omega A^s & \omega^2 - \omega_0^2 & -\frac{A^s \omega_0^2}{Q} \sin(\varphi^s) & \omega_0^2 \cos(\varphi^s) & 0 \\ -\frac{2\omega}{A^s} & -\frac{\omega_0}{Q} & -\frac{\omega_0 \omega}{Q A^s} & -\frac{\omega_0^2}{Q} \cos(\varphi^s) & -\frac{\omega_0^2}{A^s} \sin(\varphi^s) & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & -K_1 K_3 K_P d & 0 & 0 & K_1 K_3 (K_P d - K_I) \\ 0 & 0 & d & 0 & 0 & -d \end{pmatrix}$$

# Stability analysis of the linear closed looped system

Resonance condition:  $\varphi = -\pi/2$ ,  $\omega = \omega_0$

Routh-Hurwitz stability analysis  $\Rightarrow$  5 determinants :  $\Delta_1, \Delta_2, \Delta_3, \Delta_4, \Delta_5$ .  
Must be **positive** for the system to be **stable**

$\Delta_1$  and  $\Delta_2$  are unconditionally positive

